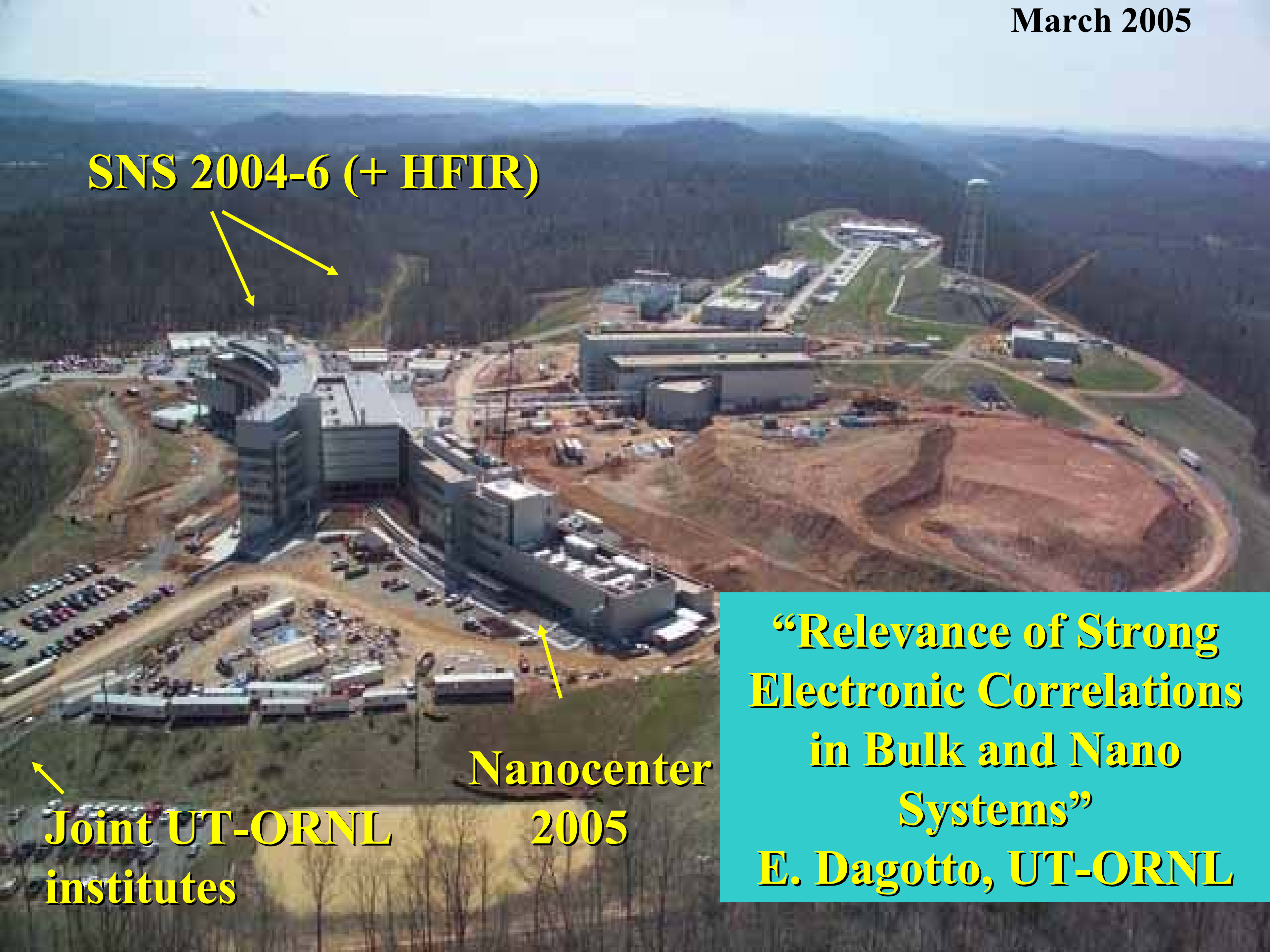
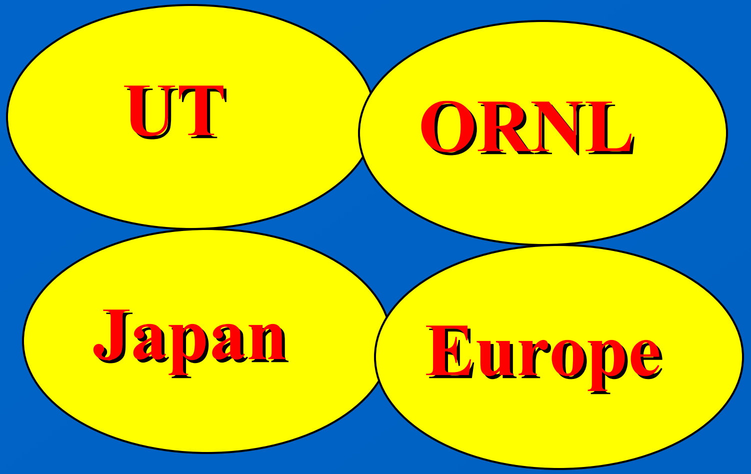

March 2005
SNS 2004-6 (+ HFIR)
Nanocenter
2005
Joint UT-ORNL
institutes
"Relevance of Strong
Electronic Correlations
in Bulk and Nano
Systems"
E. Dagotto, UT-ORNL

# Collaborators and organization

K. Al-Hassanieh (UT/FSU)
H. Aliaga (ORNL)
G. Alvarez (ORNL)
C. Busser (UT)
R. Fishman (ORNL)
N. Furukawa (Japan)
T. Hotta (Japan)
T. Maier (ORNL)
M. Mayr (UT/Germany)
A. Moreo (UT/ORNL)
Y. Motome (Japan)
T. Schulthess (ORNL)
C. Sen (FSU/UT)
I. Sergienko (ORNL)
S. Sorella (Italy)
Y. Yildirim (UT)
S. Yunoki (Italy)




1. Bulk
2. Nano

Emphasis on computational physics.

# Homework: Why having the SNS and the CNMS close to one another makes sense?

**My personal story: Recently (2004) hired by UT/ORNL as DS in CM Theory.
Expertise in computational physics, emphasizing *strong correlation effects.***

***Homework rephrased:* Why did I accept the UT/ORNL offer?**

CMSD location

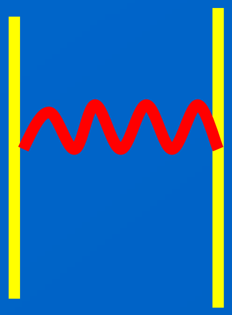
Theory offices

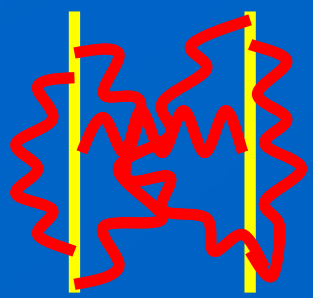
Third floor CLO/SNS

CNMS

# What are Strongly Correlated Systems?

**Strongly correlated electronic systems are those where the kinetic energy portion of the Hamiltonian is not the most important part, but the** *Coulombic repulsion and/or the electron-phonon interaction* **are.**





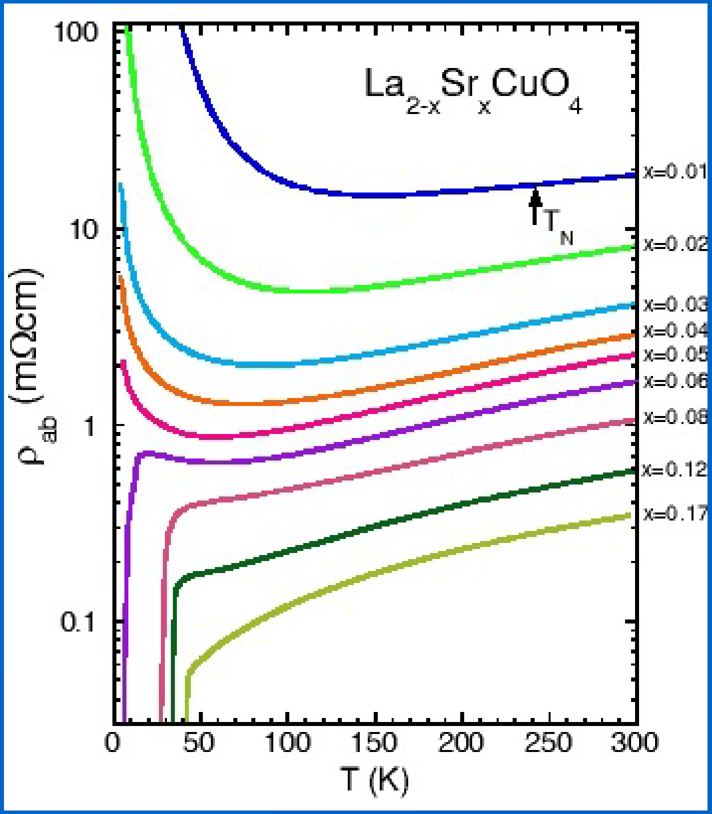
**These materials are very difficult to study both in theory and experiments!**

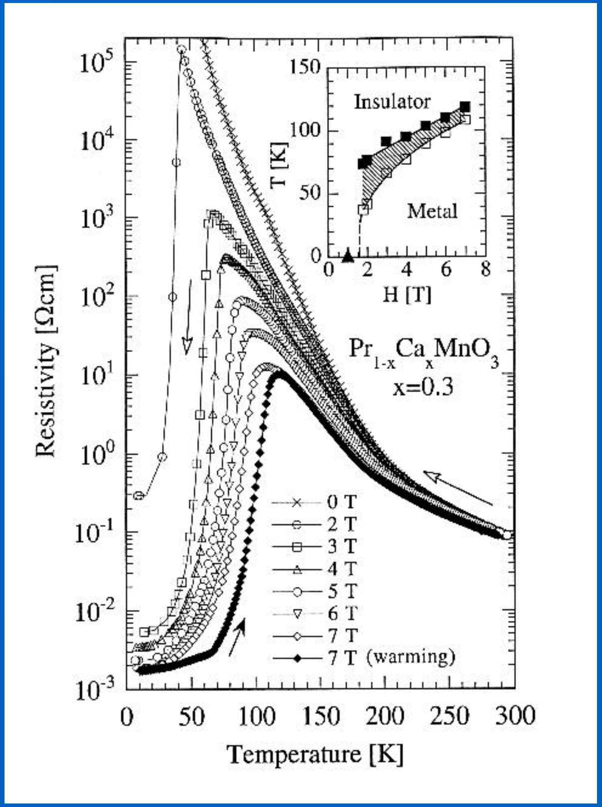
**Not only a CM problem, but the same occurs in HEP, NP,etc**

# Part I:

# Strong Correlations in Bulk Materials

# Strongly Correlated Electronic systems display a variety of interesting phenomena when in bulk form

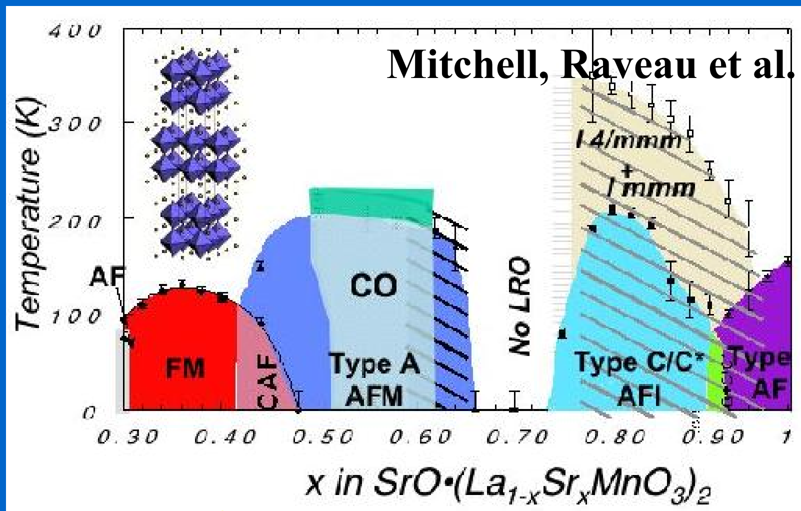


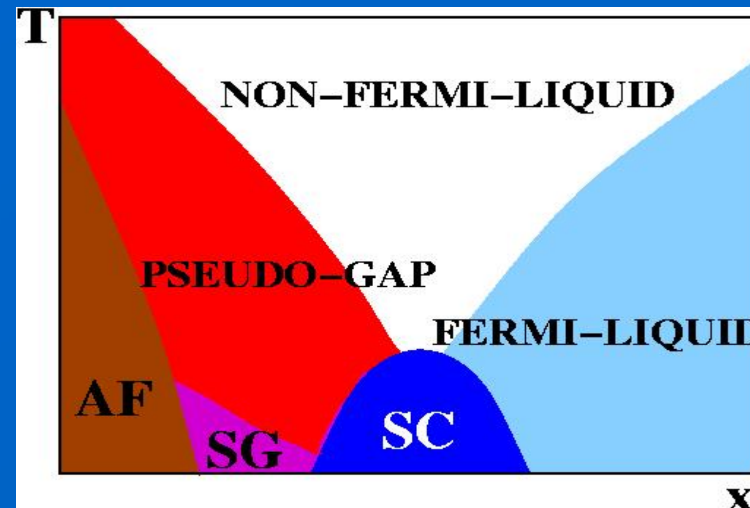

High temperature superconductors (courtesy Y. Ando)

Colossal magnetoresistive manganites (courtesy Y. Tokura)

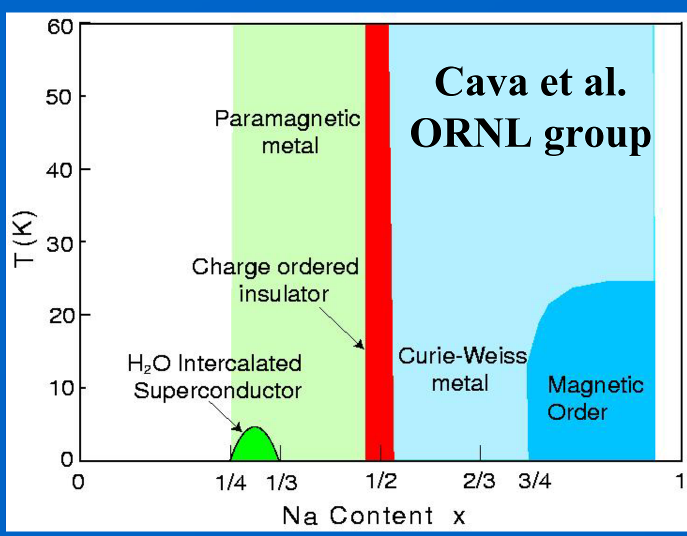
# Complex materials, phase competition



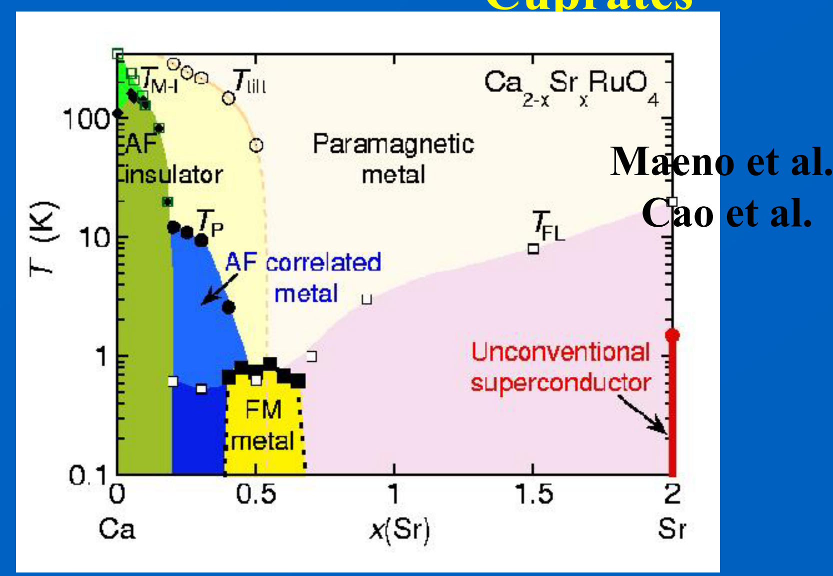

Manganites




Cuprates

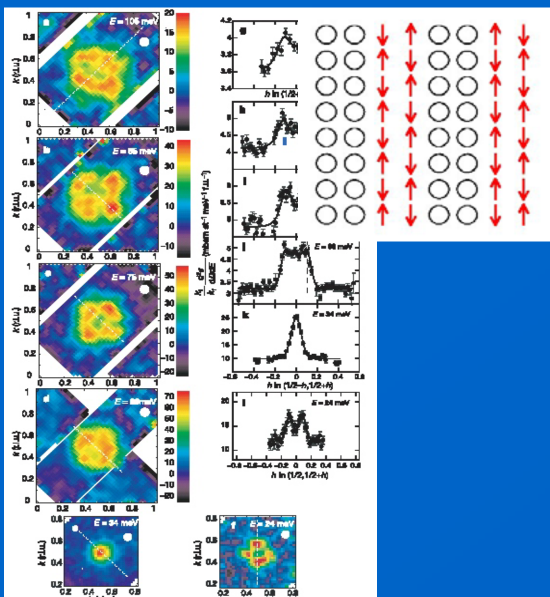



Cobaltites

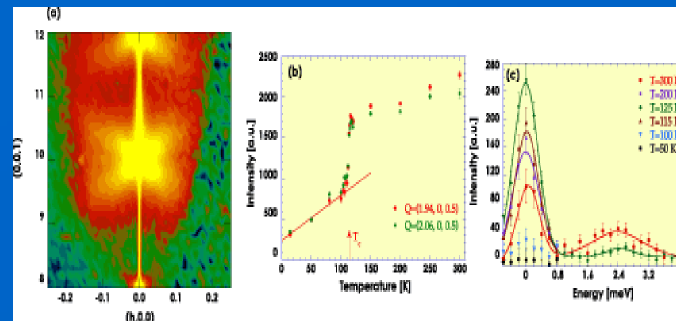



Ruthenates

# Self-organization (emergence) found in Strongly Correlated Systems.

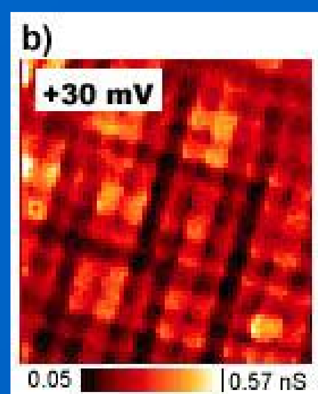


Neutrons,
Hayden et al.;
Tranquada et al.
Nature 2004 (ISIS)
STRIPES?



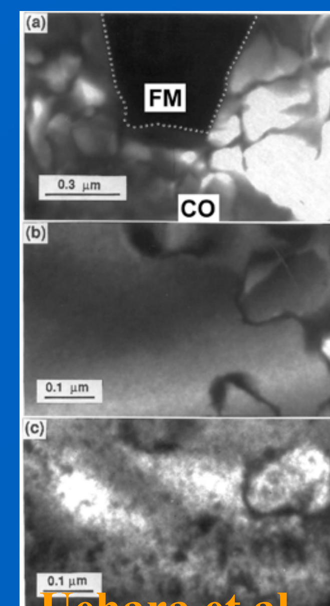

Nano-
clusters
observed

X-rays, ANL group



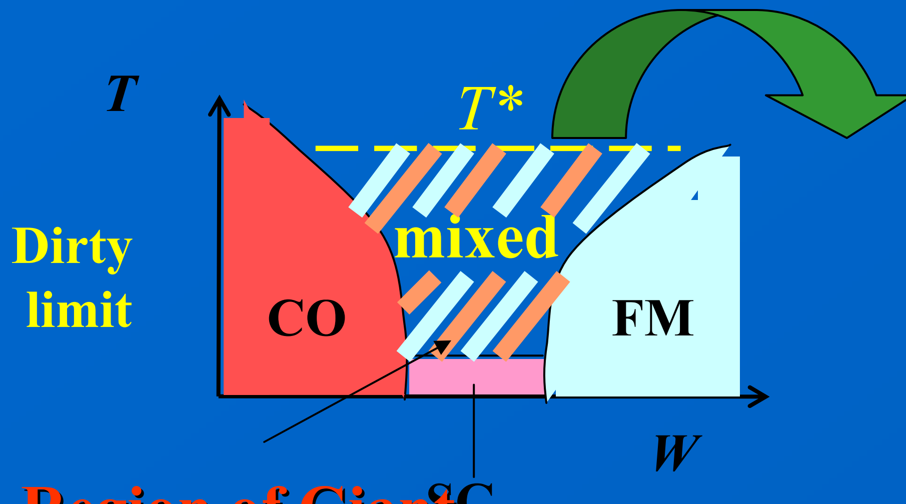

**Ca2-x Nax Cu O2 Cl2**

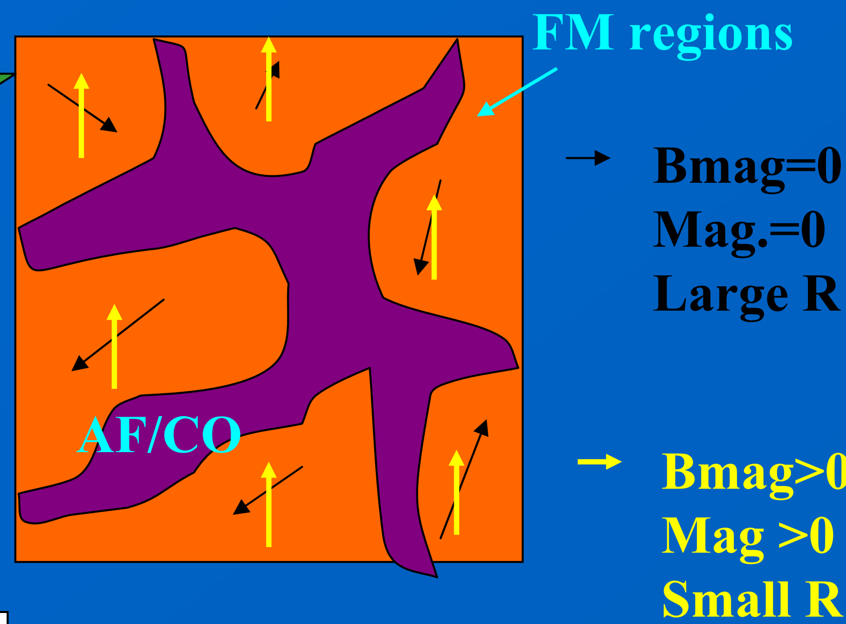
Hanaguri et al., Yazdani et al.
(Nature,Science)



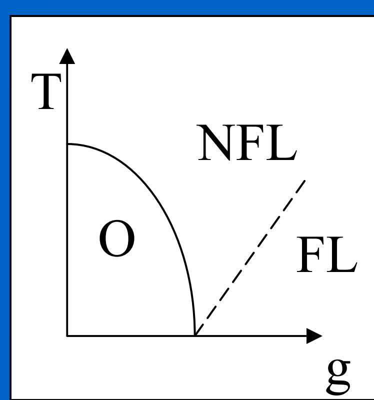

Uehara et al.,
Nature ’99

# Theory: Nanoscale separation is the origin of the CMR effect




**Region of Giant Responses (Softness)**




**High susceptibility to external magnetic fields:**
**(Science 1999, Phys. Rep. 2001)**

# Summary: A novel view of Bulk Strongly Correlated Electronic systems includes:

- **Self-organization.** Interacting units larger than atoms. Hard materials act like soft matter.
- **Giant responses**. Non-linear dynamics. Glassiness.
- Several simultaneously active degrees of freedom leads to **complexity** => nanoscale phase separation (see E.D., ``*Complexity in SCES*'', Science 05).

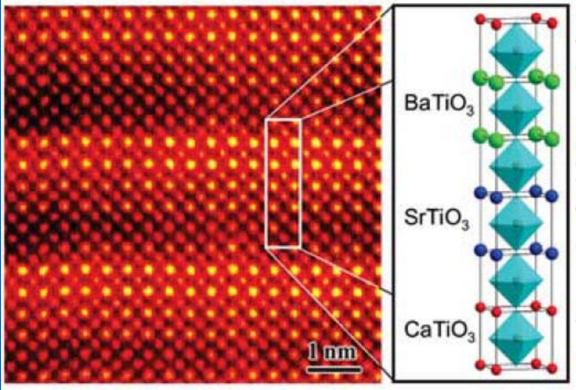
# Part II:
# Strong correlations in nanosystems.

To win big, we need to dream big!
Functionality emerging from complexity:
``Complextronics''? ``Orbitronics''?

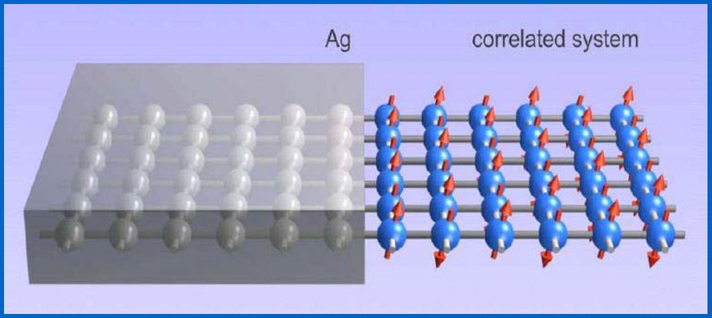
In experiments, functional complex oxides will be pursued at ORNL (Egami, Lowndes, Plummer, Shen, …) and also at BNL, ANL, …

In theory, we need further development of research area Theory of Strongly Correlated Nanoscopic Systems.

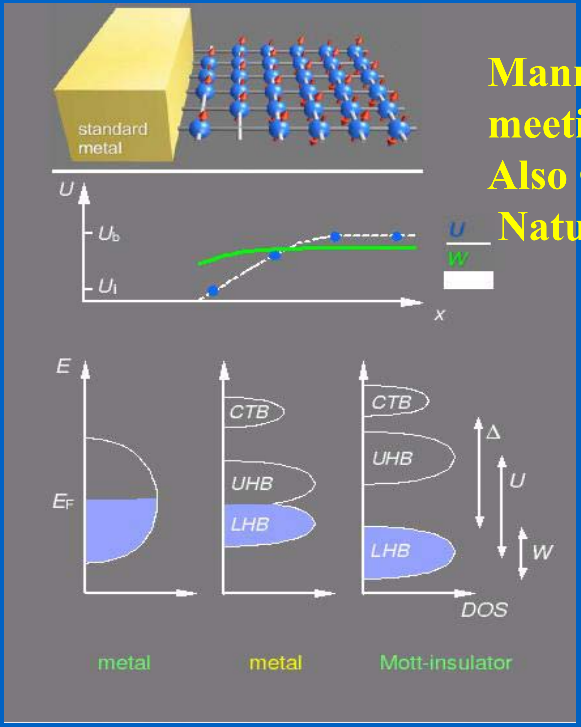
# Multilayers involving correlated systems? Applications of ``complexity'' at the nanoscale?




H. N. Lee et al., Nature 2005.
Enhancement of ferroelectricity.
Ohtomo et al., Nature 2002: metal induced between two insulators.



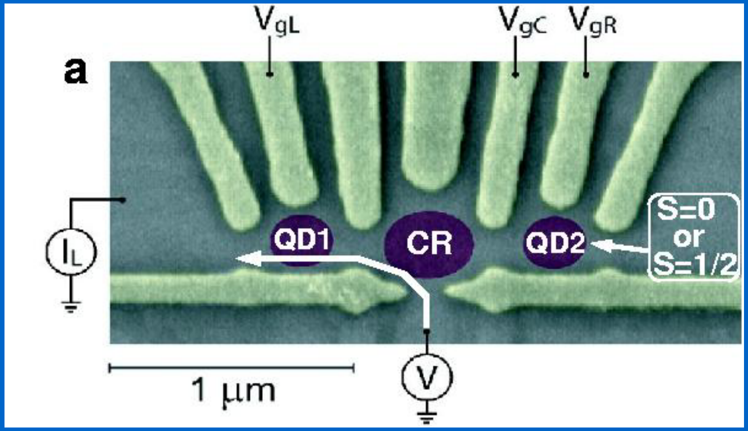

Maybe new phases can be created at the interface?



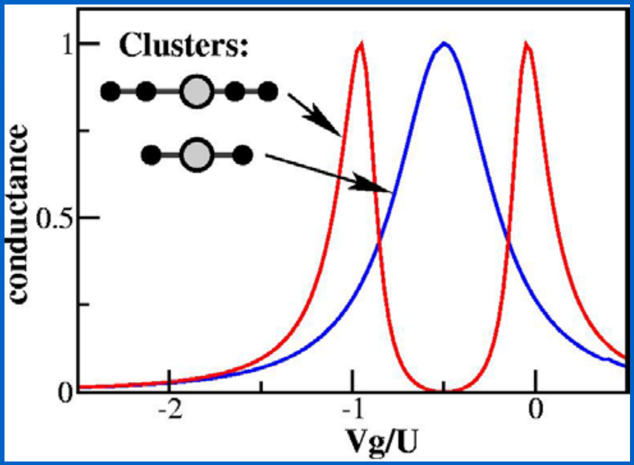

Mannhart, Dresden meeting 2005.
Also Okamoto et al., Nature 2004

Can CMR be artificially made?
Can stripes be artificially made?

# Quantum Dots and Kondo Effect

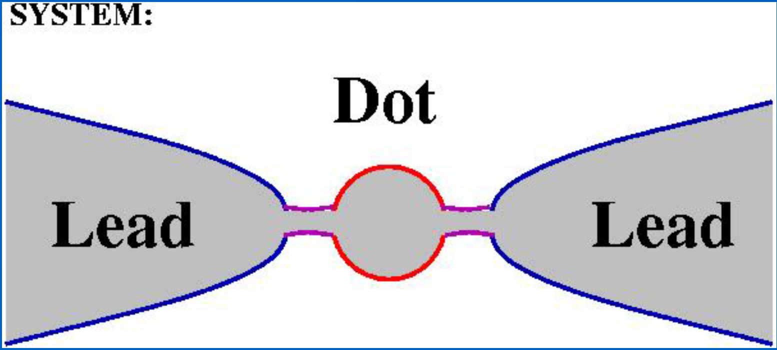



**Marcus et al., Science 2004.**




**Relation with bulk complex oxide: similar models are used, although scales are very different.**

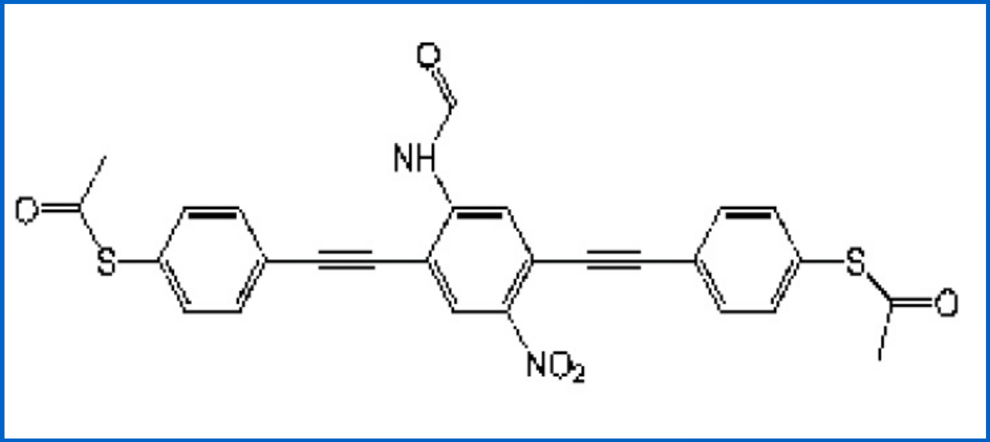
**Note: Contact with leads must be studied with ab-initio techniques.**



# Molecular conductors and correlation effects

Pioneered  by Ratner et al.

Reichert et al., APL 2003




S. Datta's group, cond-mat/0505375
Charging effects can be large in small molecules,
and Coulombic effects cannot be neglected.

# Summary 1: The Synergetic Loop


THEORY

FUNCTIONALITIES:
MULTILAYERS; DOT ARRAYS;
MOLECULAR CONDUCTORS.

NEW CONCEPTS,
NEW PHASES

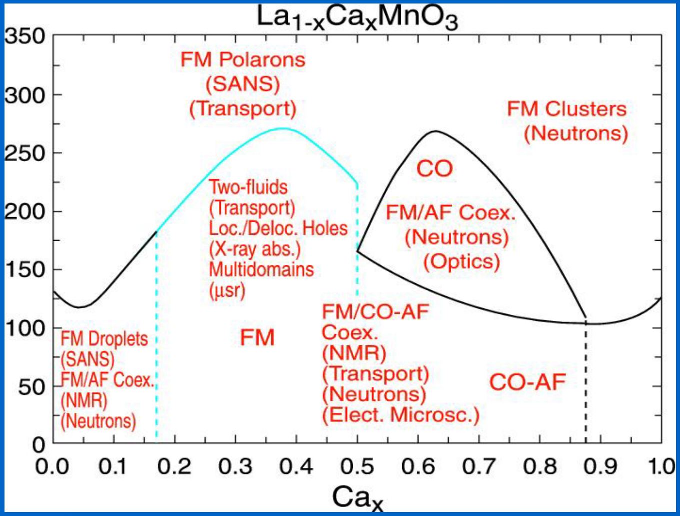
BULK STUDIES
OF COMPLEX
SCE SYSTEMS

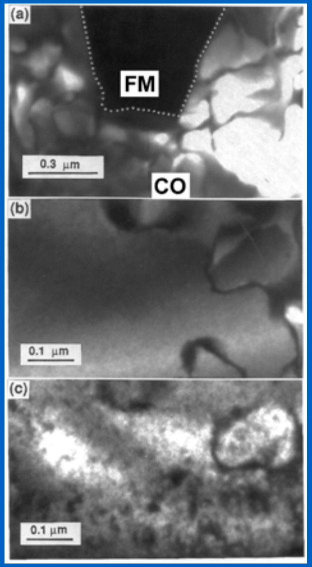
# Summary 2:  suggestions

- Higher space resolution to see nanoscale PS (better than 20-40 nm).
- Theory of Strongly Correlated nanosystems (with emphasis on computational methods) should be part of nanocenters theory goals.
- What comes next in: electronics -> spintronics --> ?    Complex SCES is a possibility.

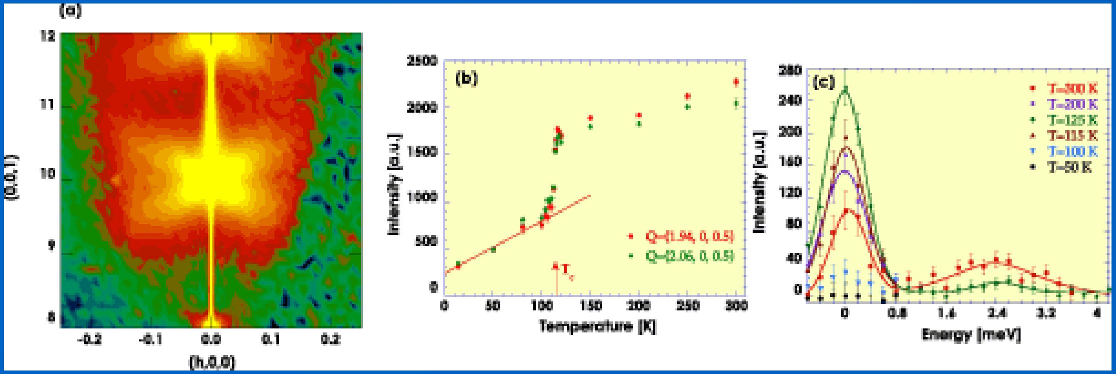
# Self-organization in CMR Manganites

A. Moreo et al., Science 283, 2034 (1999).




Uehara et al., Nature '99 LaPrCaMnO EM




Nanocluster formation observed.

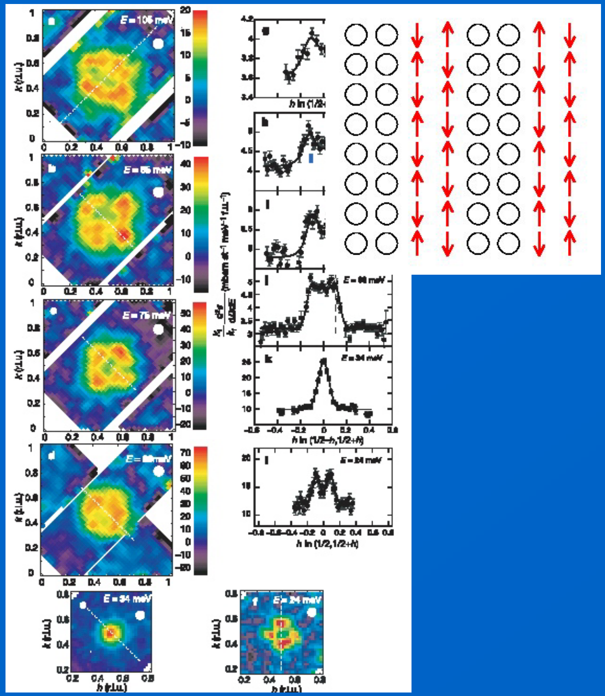
X-rays, Argonne group

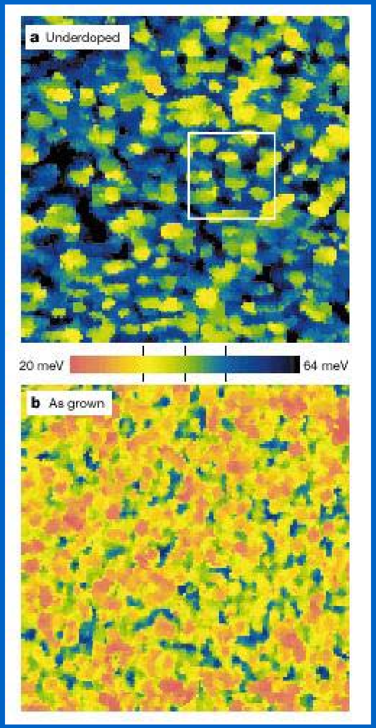
# Key Role of Computer Simulations in SCES

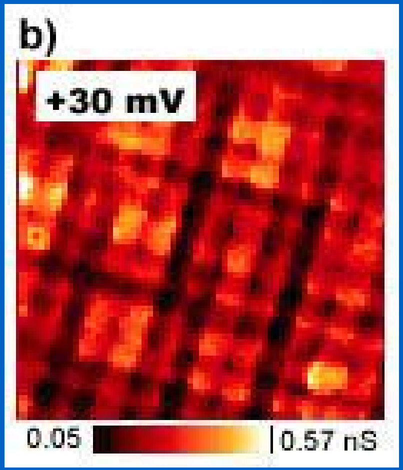
Traditional Method to search for Truffles

# Self-organization found in Strongly Correlated Systems.

CHECKERBOARD?






**Ca2-x Nax Cu O2 Cl2**

Hanaguri et al., Yazdani et al. (Nature,Science)

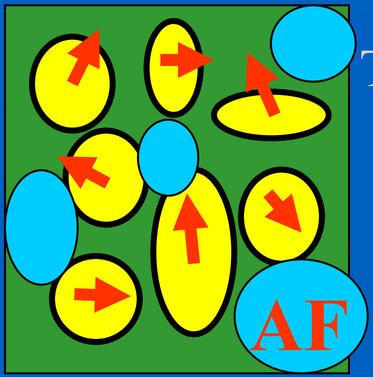
**Hayden et al.; Tranquada et al. Nature 2004 (ISIS)**

STRIPES?

**BiSCO** (Science, Hoffman et al.)

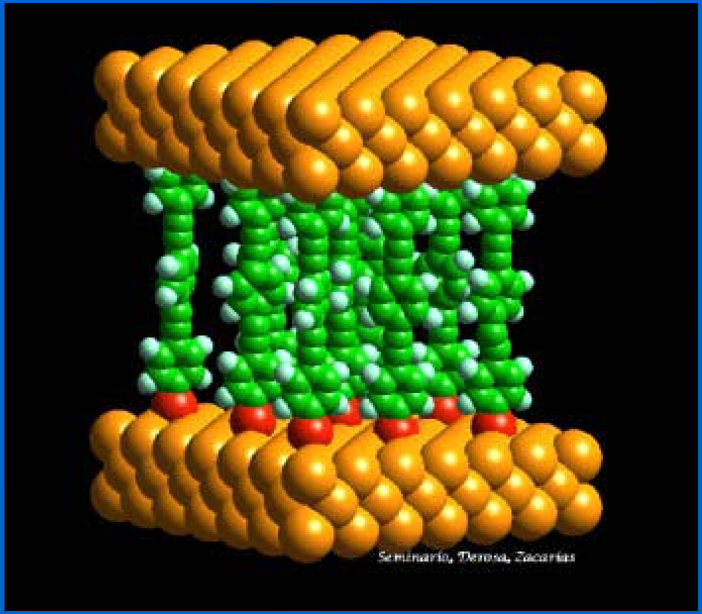
PATCHES?

Oxygen randomness?

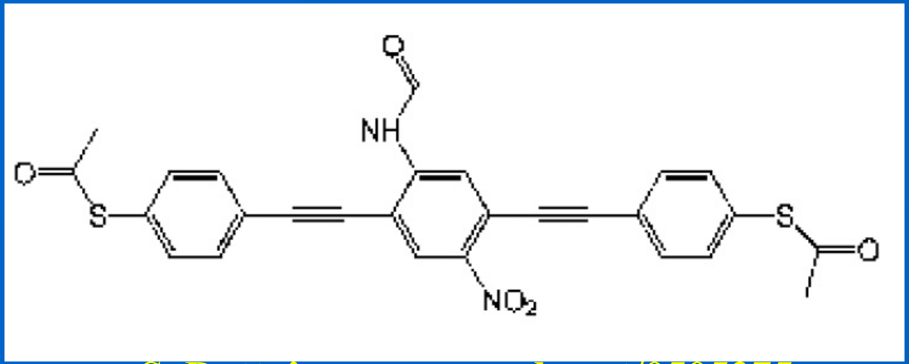



Theory

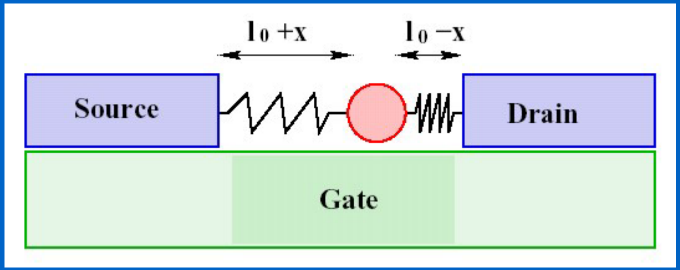
# Molecular conductors and correlation effects

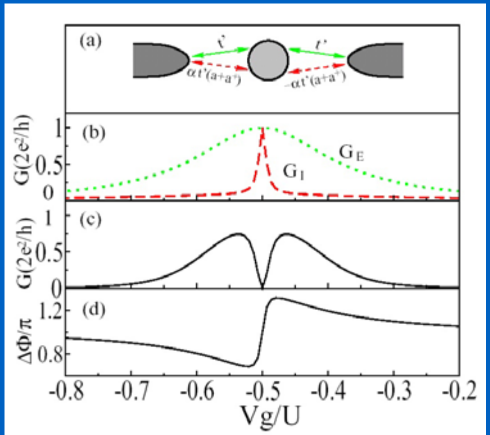



Reichert et al., APL 2003




S. Datta's group, cond-mat/0505375
Charging effects can be large in small molecules, and Coulombic effects cannot be neglected.




Goal: understand fundamental aspects of transport in small molecules
K. Al-Hassanieh et al., cond-mat/0504528

# Strong Correlation and SNS-CNMS synergy

SNS

Condensed Matter Division
Theory and Simulation of
Strongly Correlated Systems

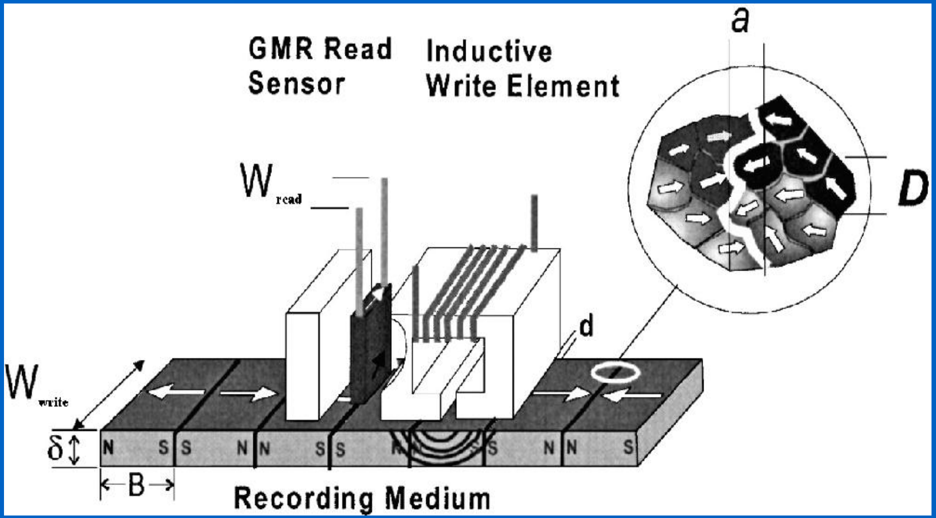
CNMS

**The study of bulk complex oxides with neutron scattering provides key information to understand/predict nanoscale systems with interesting properties. The inverse will also hopefully be true.**
**LOCAL PHYSICS IS CRUCIAL.**

# Applications possible, basic science interesting.

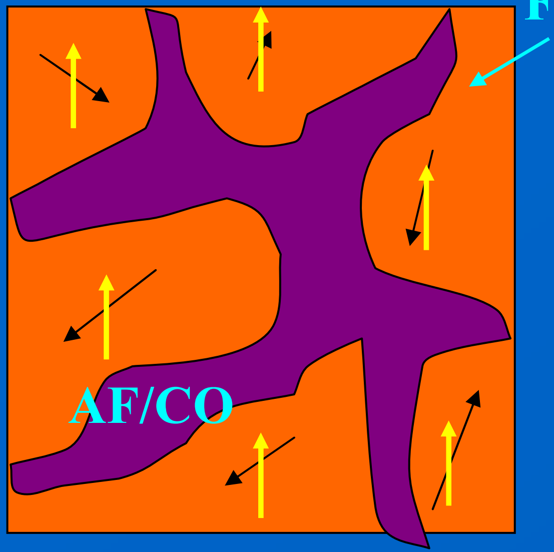
Big dreams!

(1) SC transmission lines
(2) SC energy storage
(3) Magnetically levitated trains
(4) Magnetic resonance image




Potential applications in read sensors.

# Can we artificially nano-construct the building blocks of bulk materials?



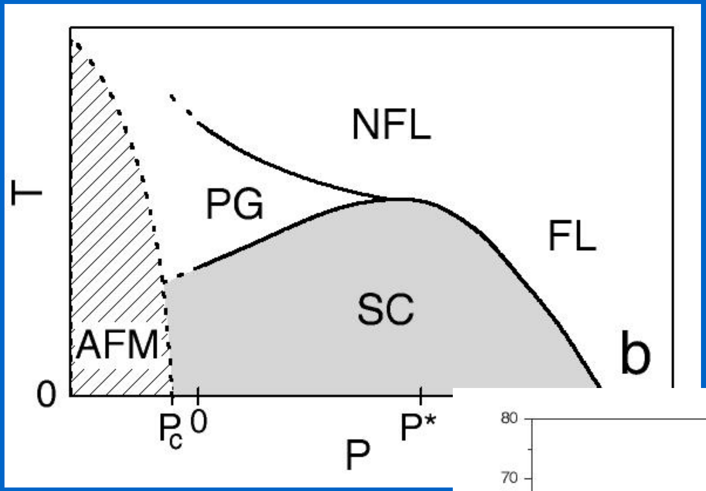

→ Bmag=0
Mag.=0
Large R

→ Bmag>0
Mag >0
Small R

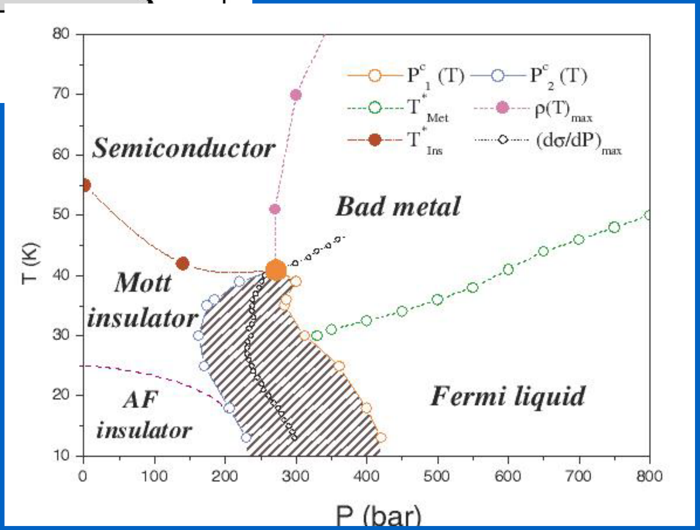
High susceptibility to external magnetic fields

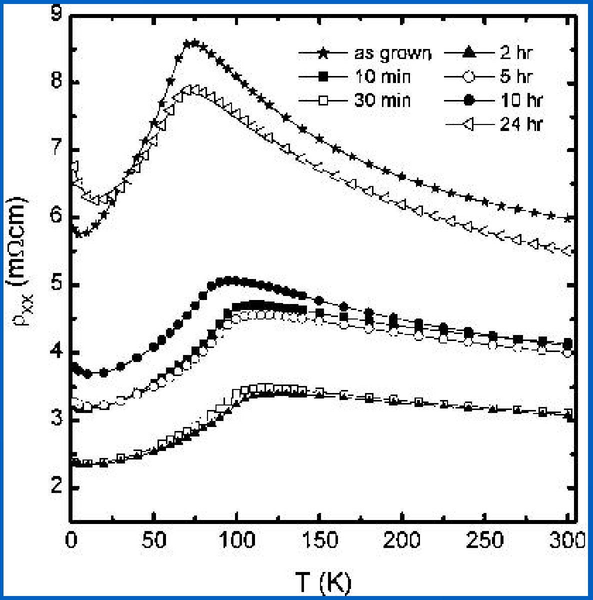
Challenge:
Can CMR be artificially made?
Can stripes be artificially made?

# Other materials where complexity may matter as well …




**Heavy fermions (LANL group)**

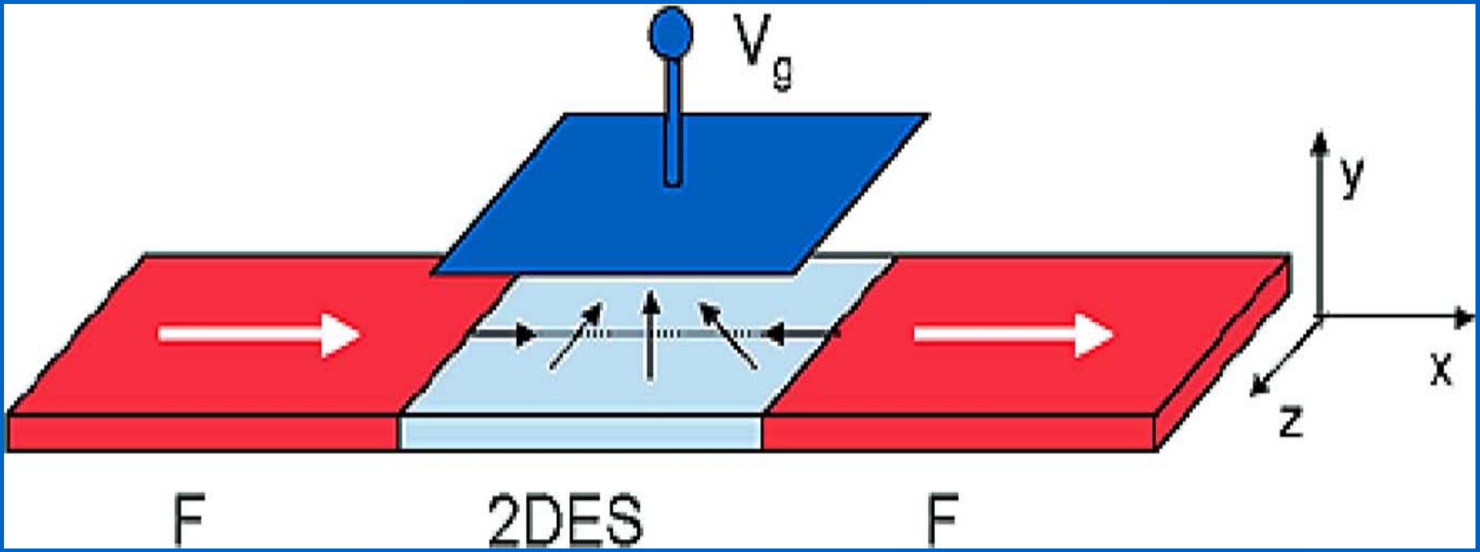



**Diluted Magnetic Semiconductors (Penn State group)**

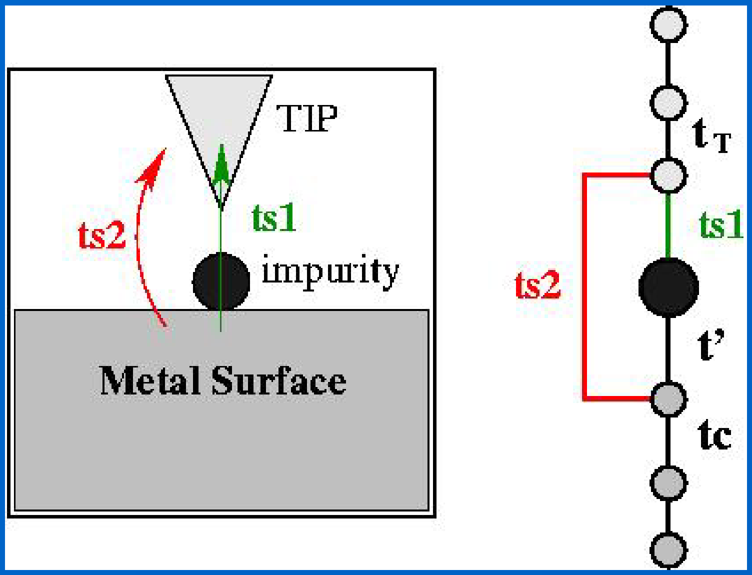
**Organic superconductors (Orsay group)**

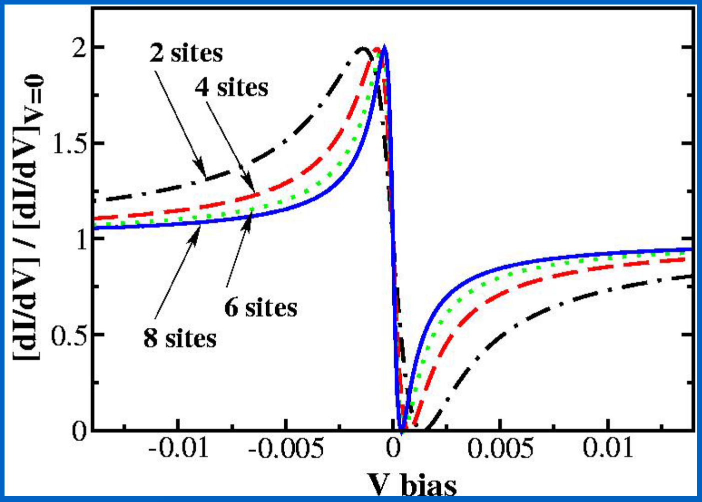
# Spin-polarized field-effect transistor (Datta and Das)




Electric field seen as magnetic field by mobile electrons

# Fano Resonances and STM

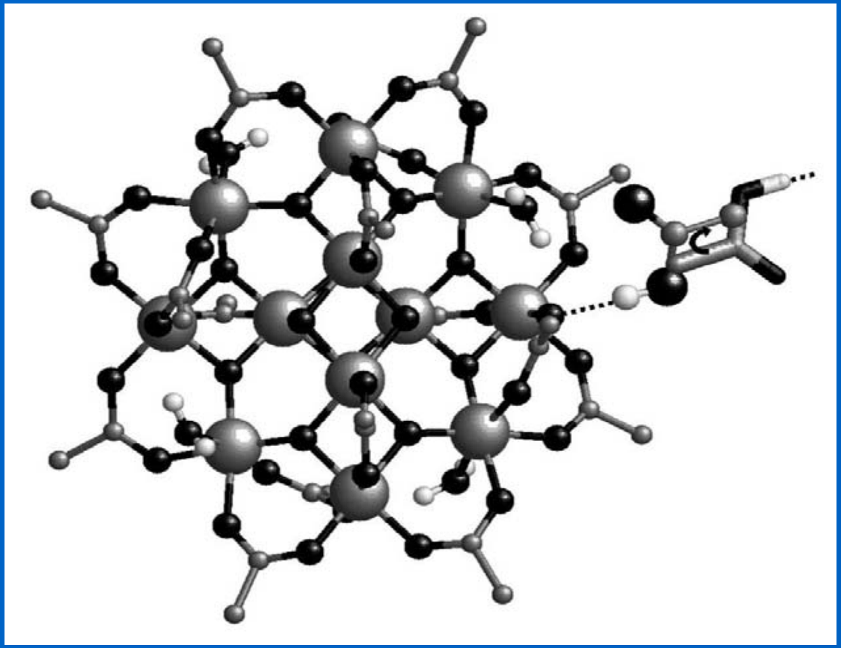



Geometry and computational setup

Results in qualitative agreement with experiments

# Nanoclusters

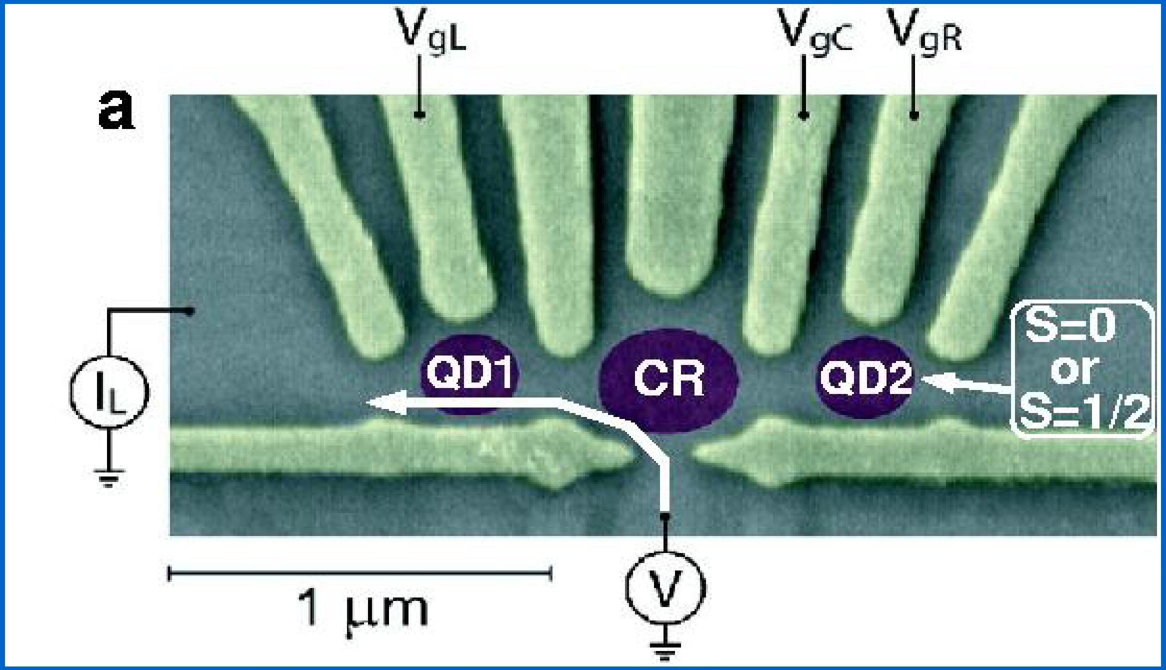


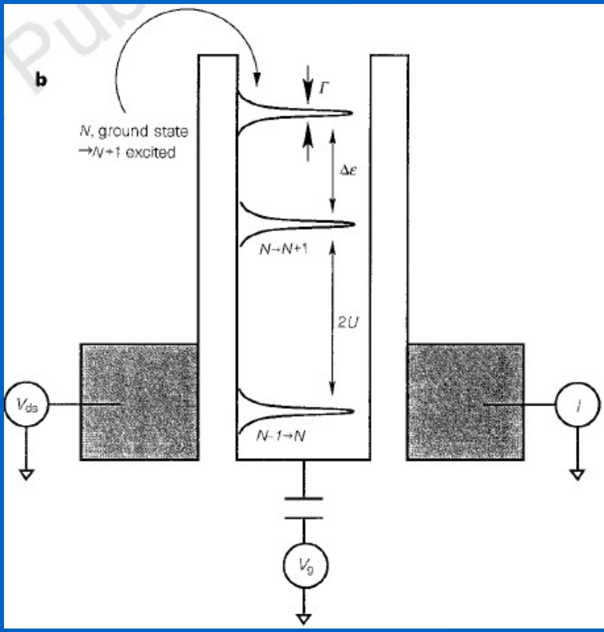

S=10, strong uniaxial anisotropy

Quantum Tunneling

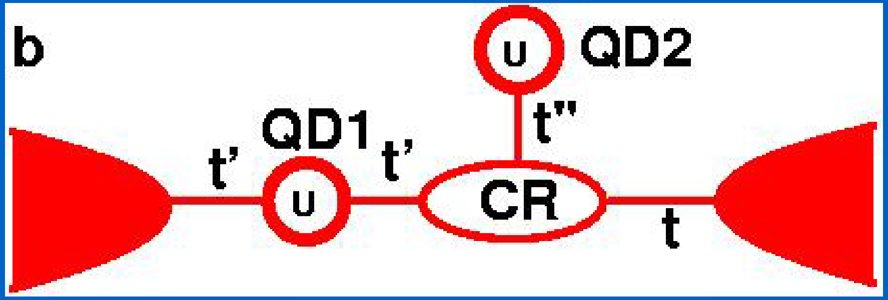
Mn12-Acetate

# Other quantum dots:

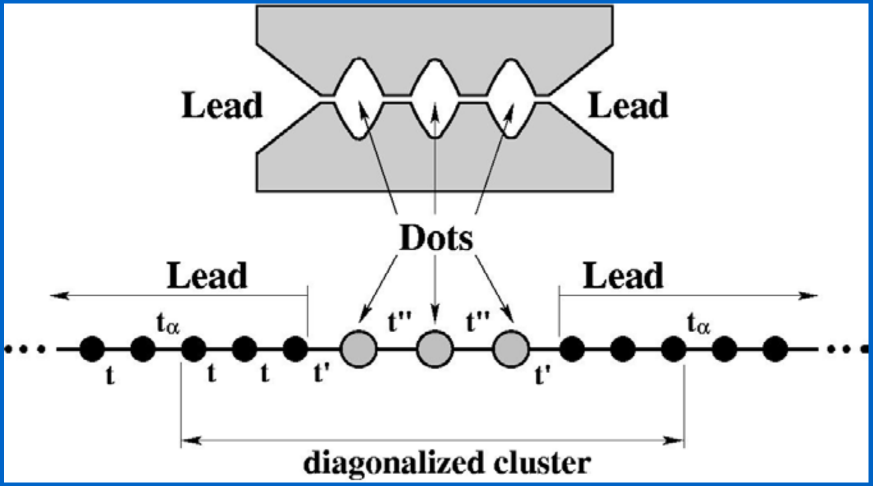


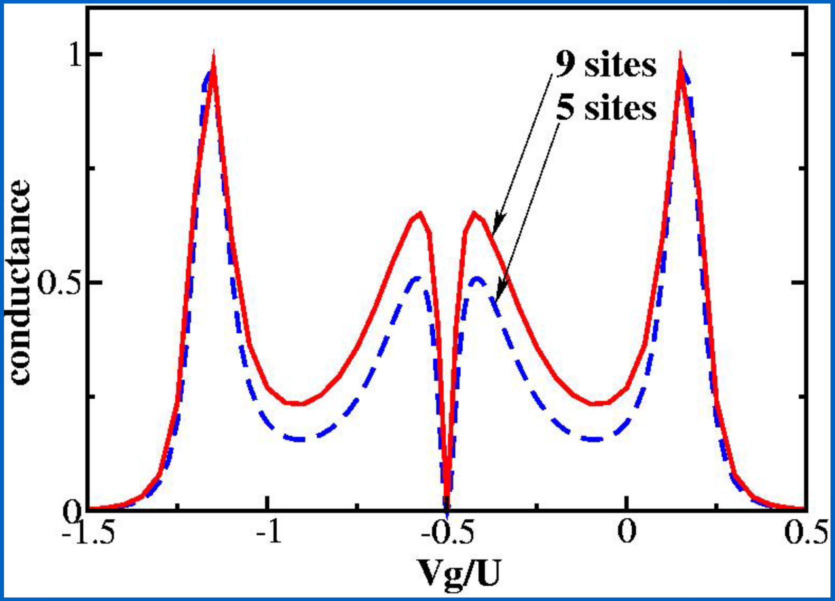

Marcus et al., Science 2004



# Quantum Dots and Correlation Effects

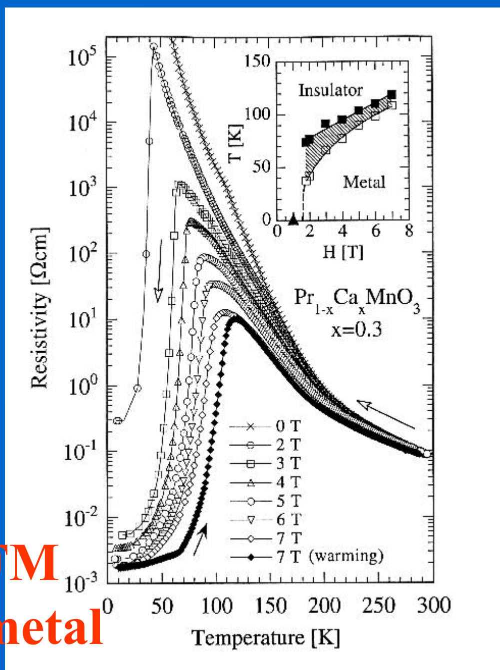



Computational setup



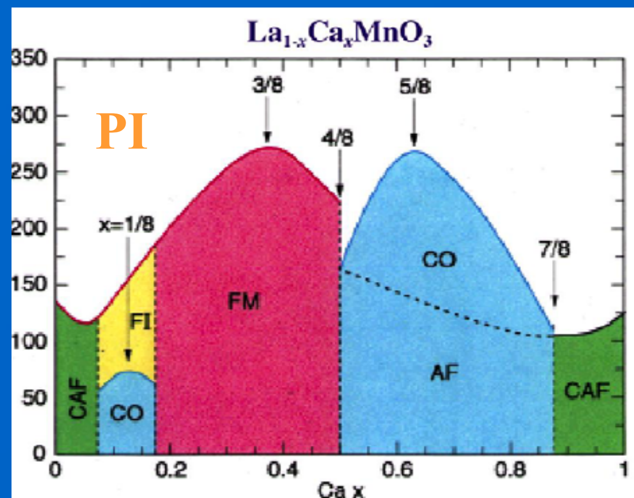

Anomalous cancellation of conductance

# (I) CMR manganites:



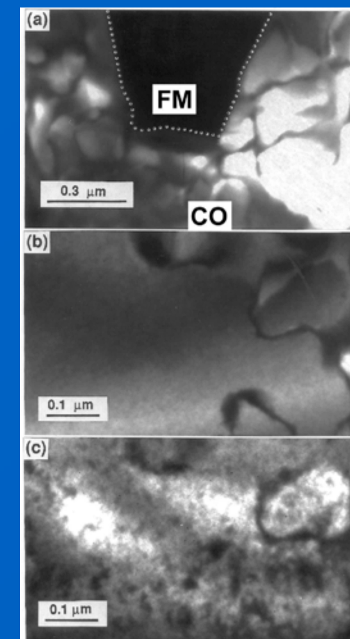

FM metal

Colossal Magnetoresistance




PI

Rich phase diagram, several states competing. Common feature of many Strongly Correlated Electronic systems.

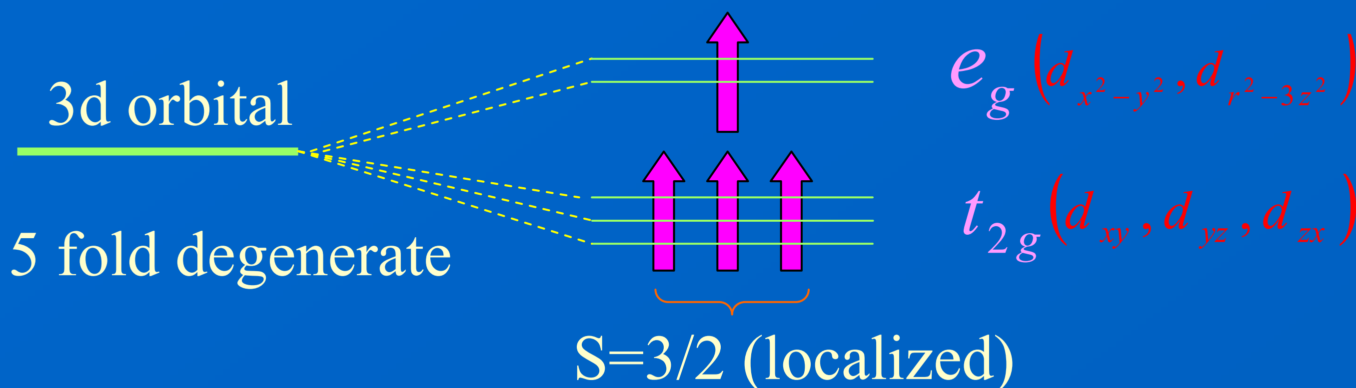



Intrinsic inhomogeneities

Uehara et al., Nature ’99 LaPrCaMnO EM

# ``Standard'' theoretical models

*Double Exchange:* fermions interacting with classical localized spins



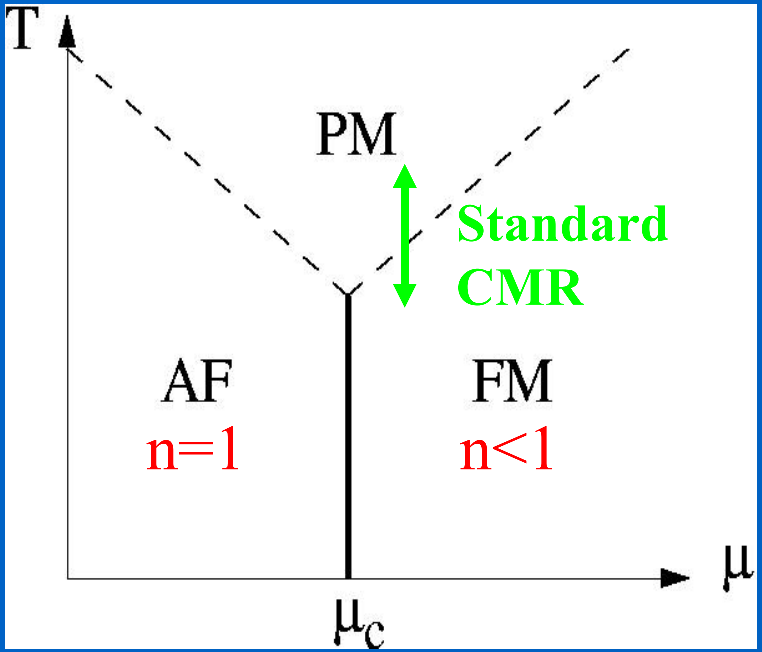

phonons

$$Z = \int DQ \int DS\, \overbrace{tr_{e_g}\left(e^{-\beta H}\right)}^{e_g \text{ electrons}}$$

$t_{2g}$ spins

# Summary of MC/MF Results
## (without quenched disorder)

- FM, AF /CO, and Electronic Phase Separation are observed. All experimentally-observed ordered phases have been found/predicted.

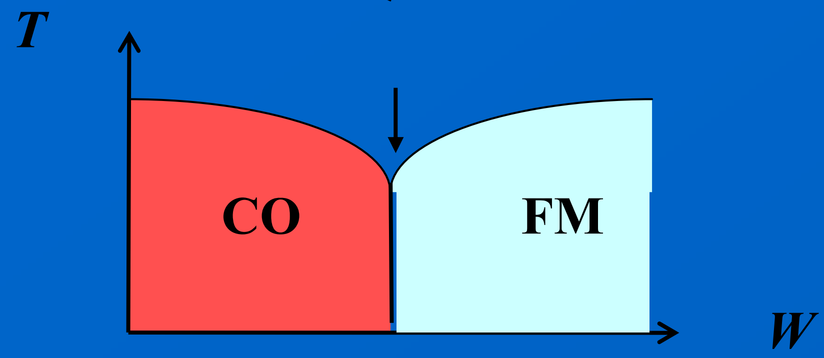



Yunoki et al. 1998.
E.D. et al., Phys. Rep. 344, 1 (2001); A. Moreo et al., Science 1999.

**First-order transitions separate FM from AF states, at different or equal electronic densities.**

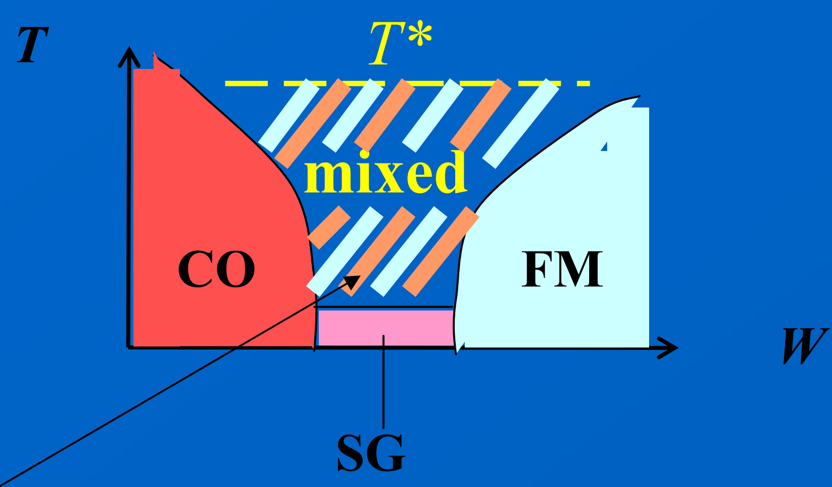
# CMR theoretical explanation: Phase Competition in the Presence of Quenched Disorder

clean



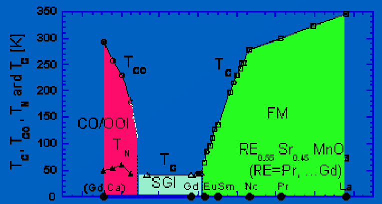

Burgy et al., PRL87, 277202 (2001).
See also Nagaosa et al. and Salamon et al..

dirty

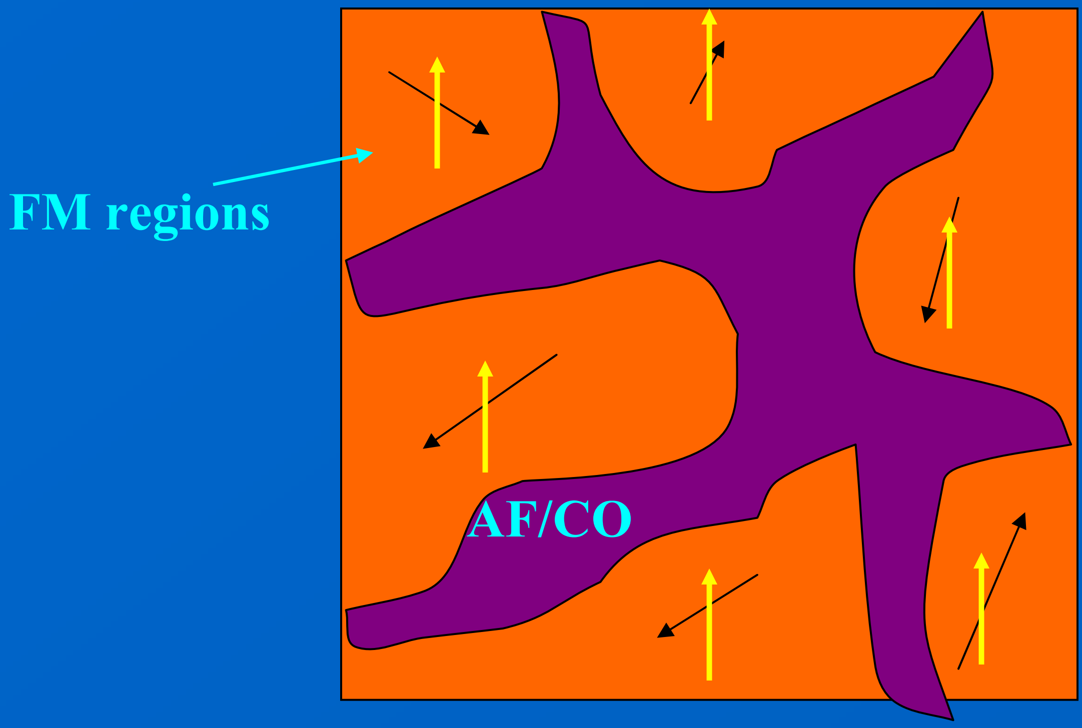



**Region of Giant Responses (Softness)**

**For experiments see Akahoshi et al. PRL 2003 Tomioka and Tokura, PRB70, 014432 (2004).**



# Manganite CMR State
# in the ``mixed'' regime




Magnetic Field=0
Magnetization=0
Large R

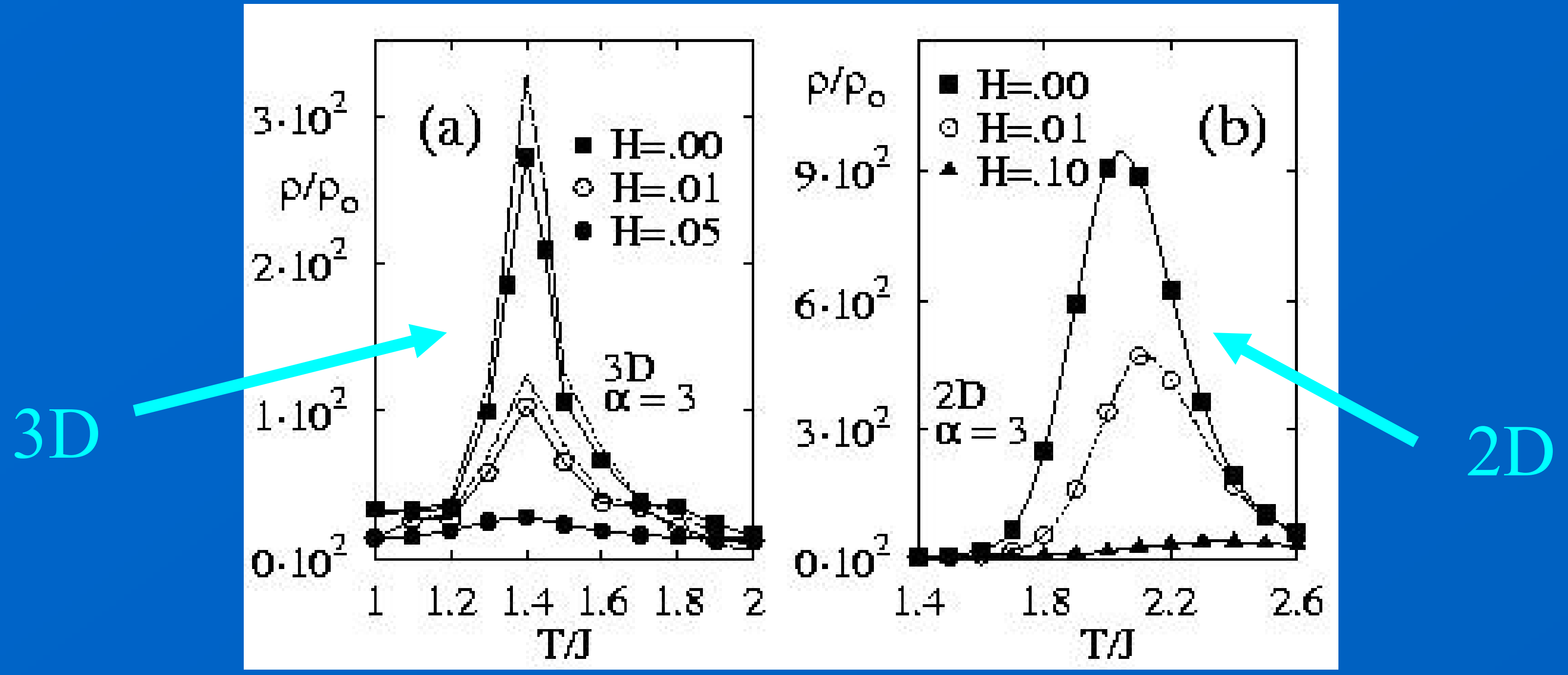
Magnetic Field>0
Magnetization >0
Small R

**High susceptibility to external magnetic fields: rapid rotation of preformed nano-moments**

(Phys. Rep. 344, 1 (2001); see also S. Cheong et al.)

# MC for a ``Toy Model'' with correlated disorder to mimic cooperative JT effects

(J. Burgy et al., PRL92, 097202 (04); A. Bishop, T. Egami et al.)

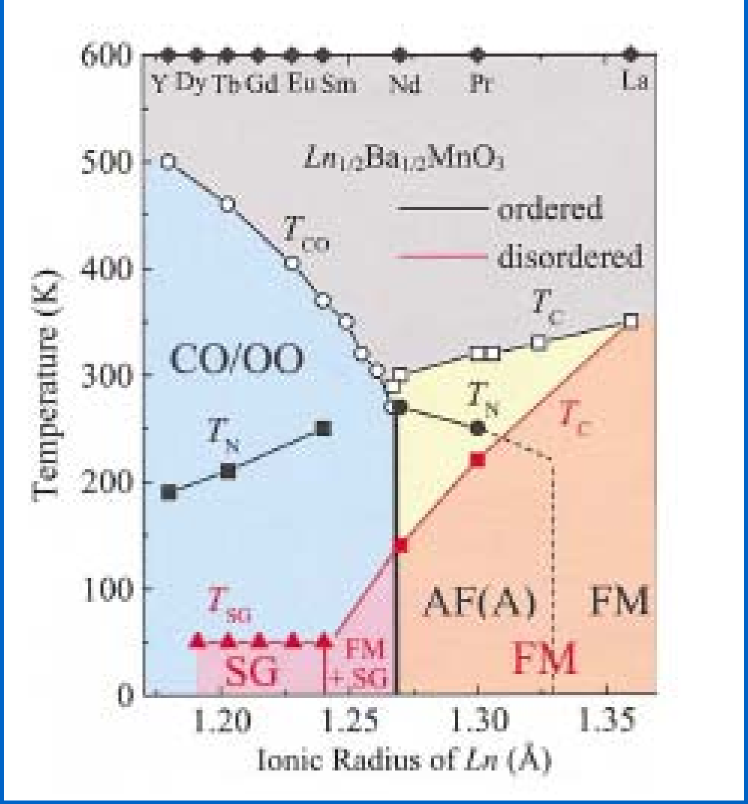


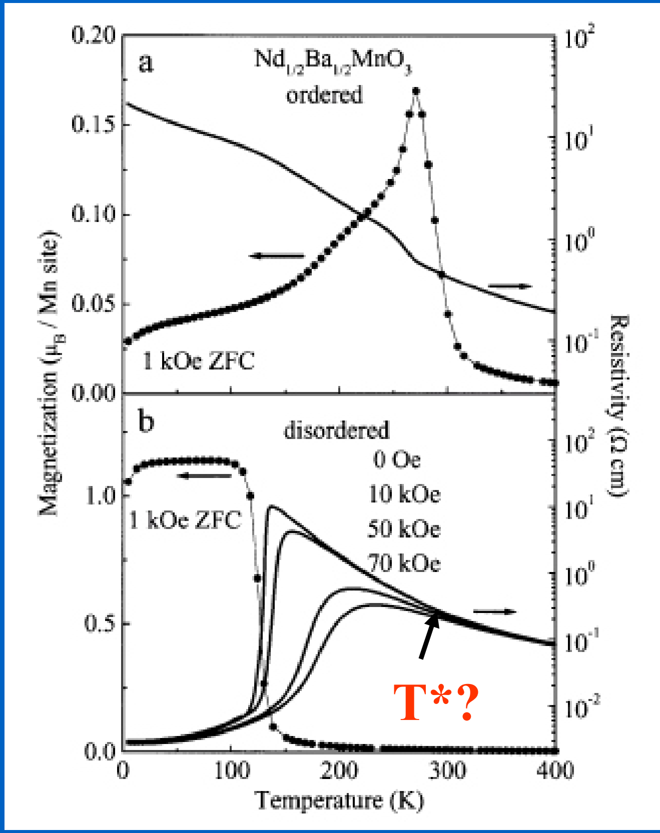

**3D and 2D are very similar.**

**Disorder strength needed goes down as disorder correlation length increases.**

# Experiments controlling quenched disorder are very important

RE(1/2)Ba(1/2)MnO3; Akahoshi et al., PRL 90, 177203 (2003)



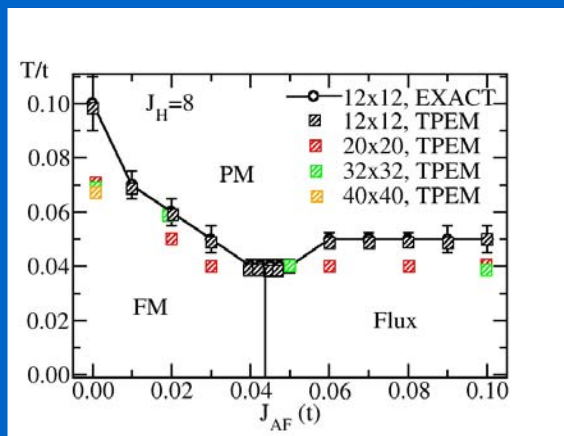




**Without ``dirt'' the CMR effect does not occur!**

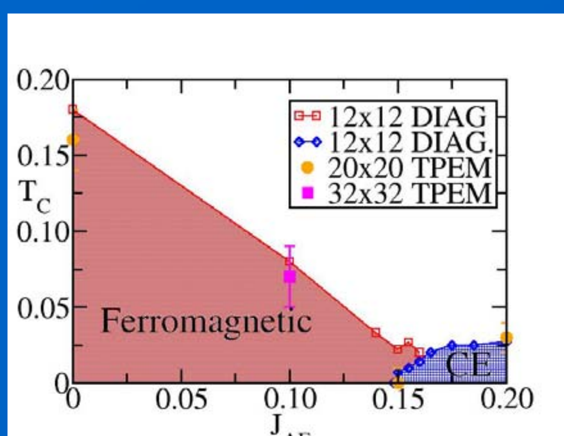
# GRAND CHALLENGE PROJECT:
## Large clusters using Double Exchange models can be studied using a new method ( TPEM, Truncated Polynomial Expansion method, Furukawa and Motome)

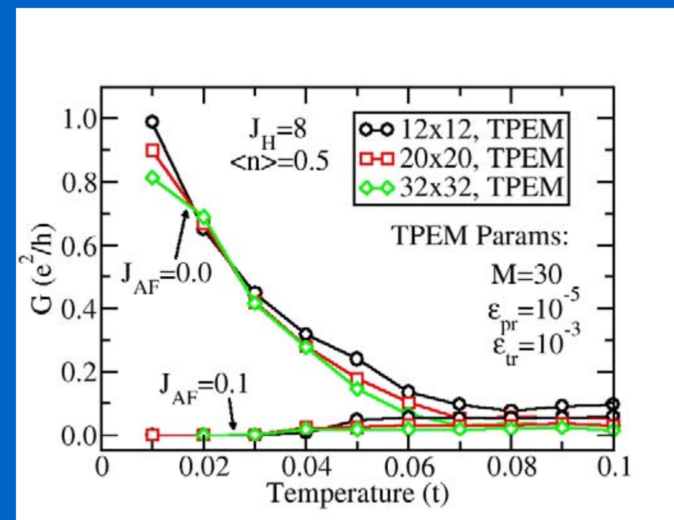
conductances

1 orbital
(C. Sen)




2 orbitals
(Alvarez,
Sergienko)



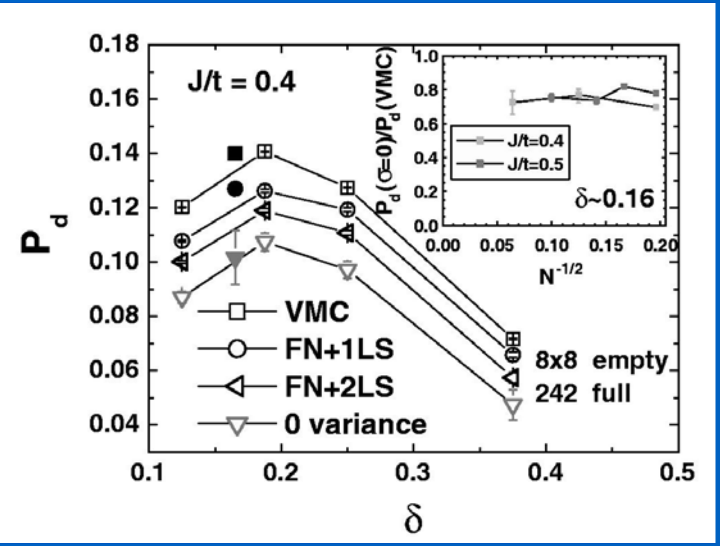

Order N method: DOS expanded in Chebyshev polynomial, localized electron basis, local nature of MC updates, and sparse Hamiltonian
(Alvarez et al., cond-mat/0502461)

# (II) High-temperature superconductivity

Sorella et al., PRL 88, 117002 (2002)

- **Hubbard and t-J models computational studies *are reaching the limits of what can be done.* Fortunately, dominant tendencies have been identified.**

E.D., RMP 66, 763 (1994)



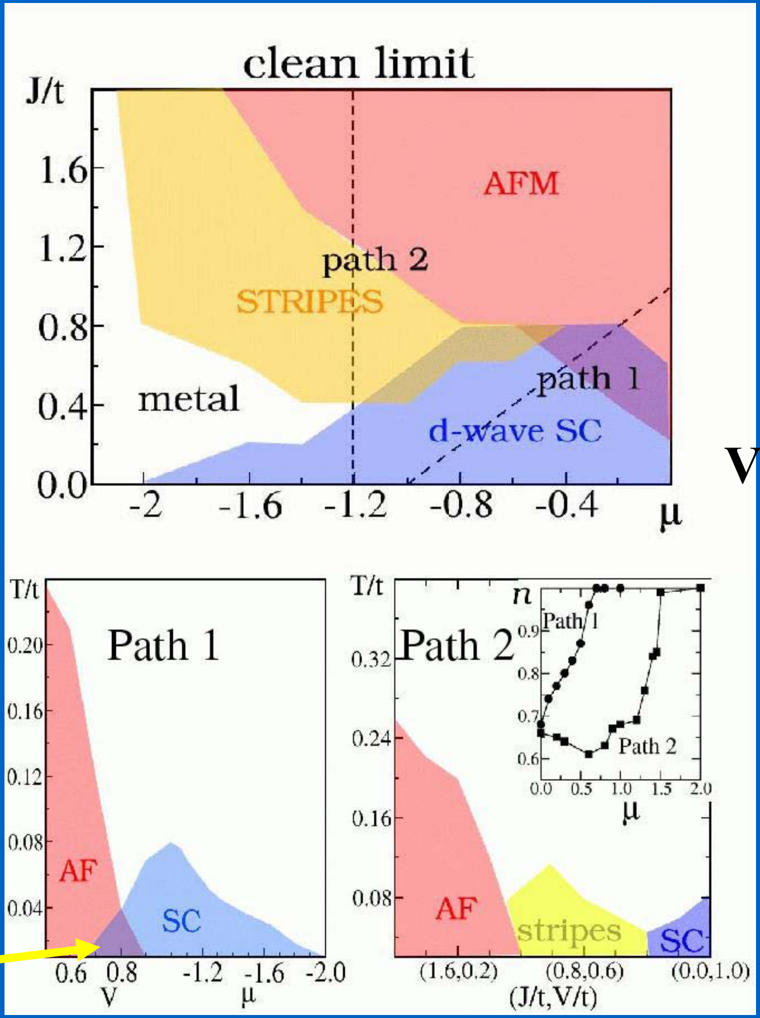

**SC appears in t-J simulations due to short-range AF, as in 2-leg ladders**
**However, other studies show stripes (Scalapino+White,etc).**
**Once again, several phases in competition.**

# Complexity in high-Tc?
# Phenomenological SC vs. AF competition

**Monte Carlo results for ``mean-field-like'' model of mobile electrons coupled to classical AF** (Moreo et al., PRL 88, 187001 (2002)) **and SC order parameters** (Alvarez et al., PRB 71, 014514 (2005)).

Two parameters: J and V.

Technically: MC approximations can be used after Bogoliubov transformation (Hirschfeld)



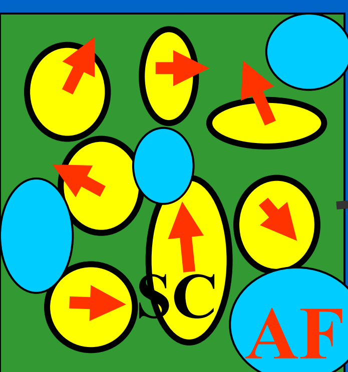

V=1-J/2

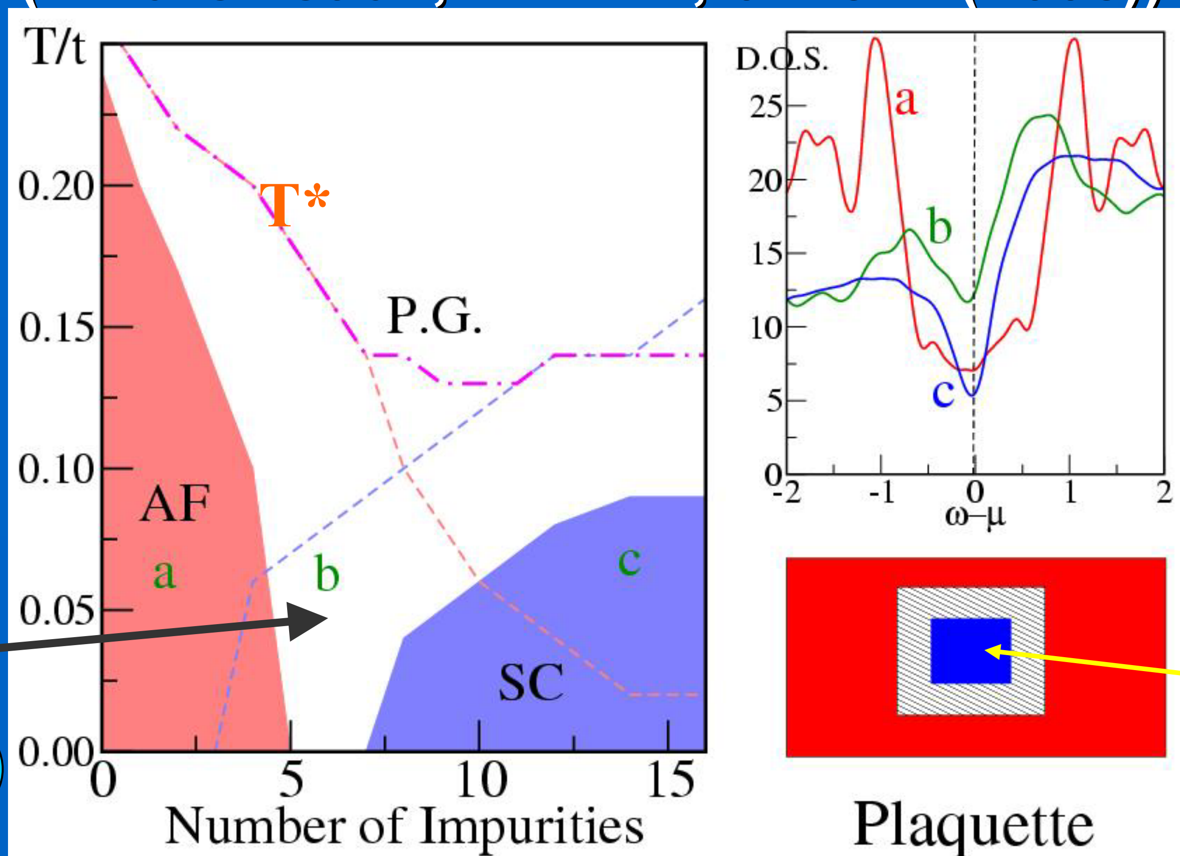
Local coexistence

## Results similar as in Mn-oxides predicted for high-Tc:

# Quenched disorder leads to glass, clusters and T*, as in manganites

**(Alvarez et al., PRB 71, 014514 (2005)).**



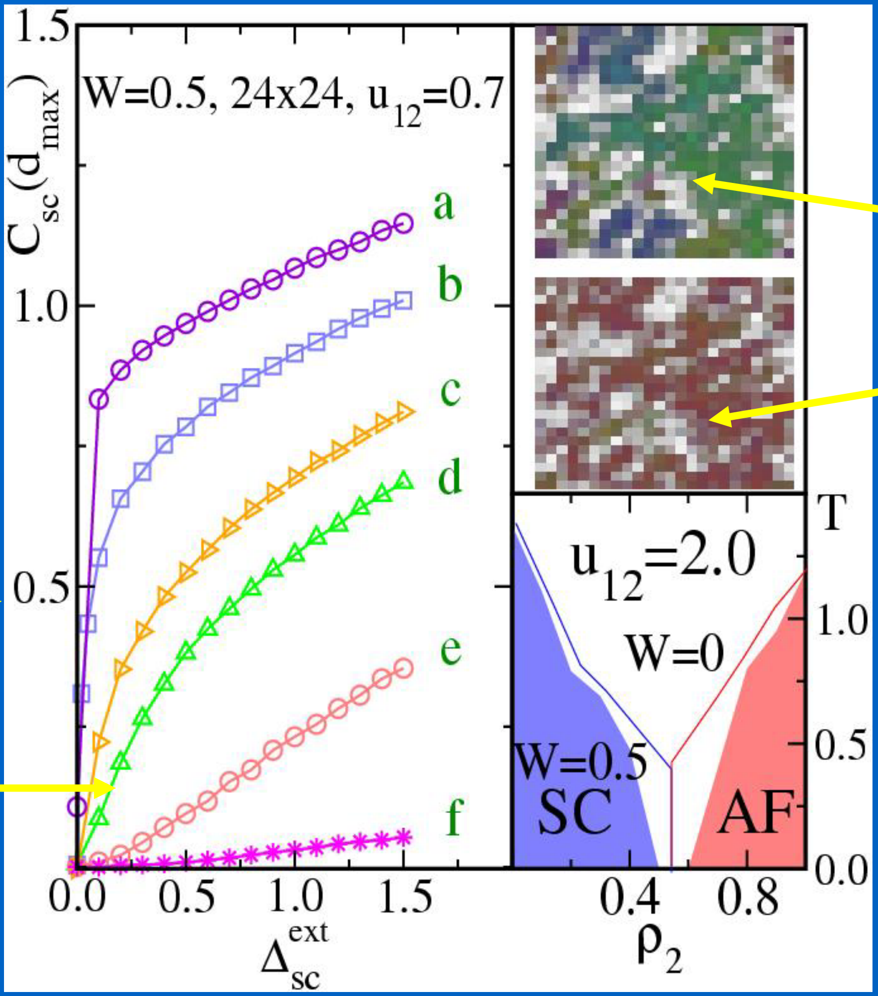



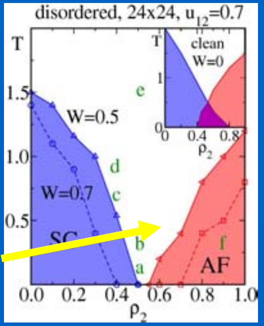

Coulombic centers, as in Sr++. Each provides 1h.

$\Delta=|\Delta|\, e^{i\phi}$

# Giant effects in high-Tc?

**(Alvarez et al., PRB 71, 014514 (2005)).**



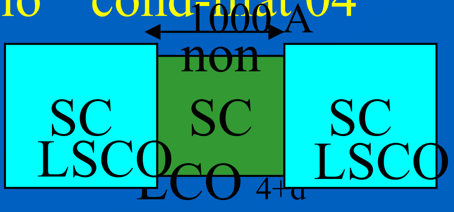

``non-SC glass''
(colors<->angles)

``Inhomogeneous''
superconductors

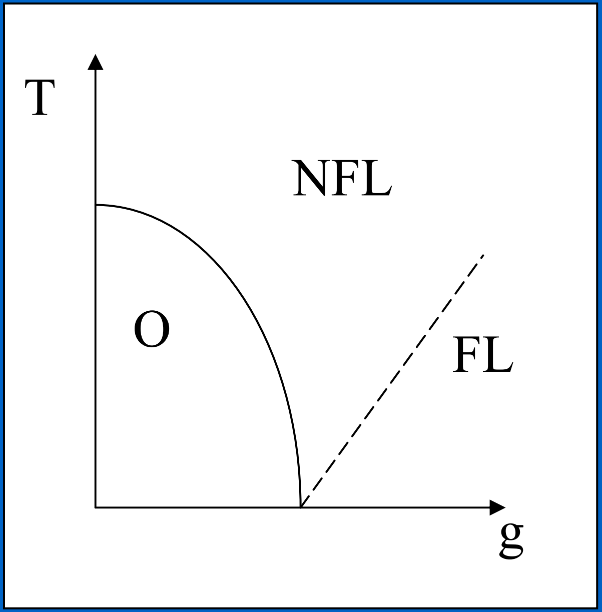
High
susceptibility
to ``external
SC fields''

**"Colossal" Effects in underdoped regime?**

(``Giant proximity effect''
Bozovic et al. PRL 04).
Homes et al.: ``dirty SC
scenario'' cond-mat 04

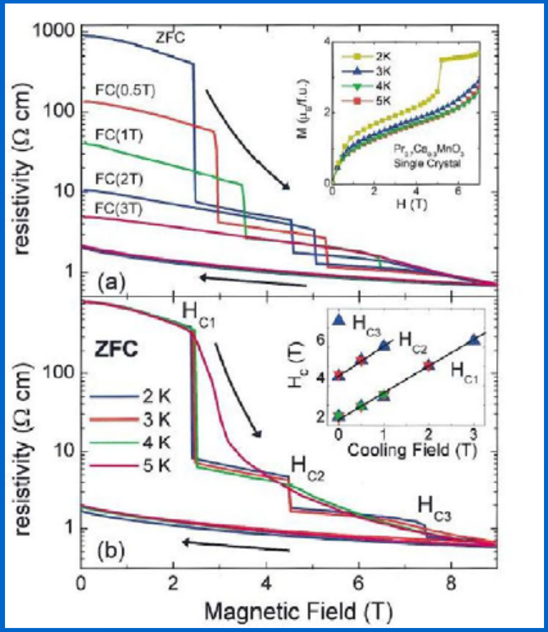


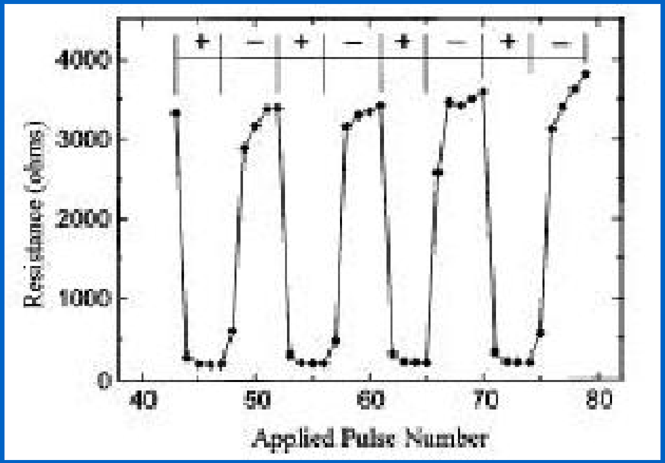
*To be discussed:* **generalization to the case of QCP and competition ordered phase vs. metal.**

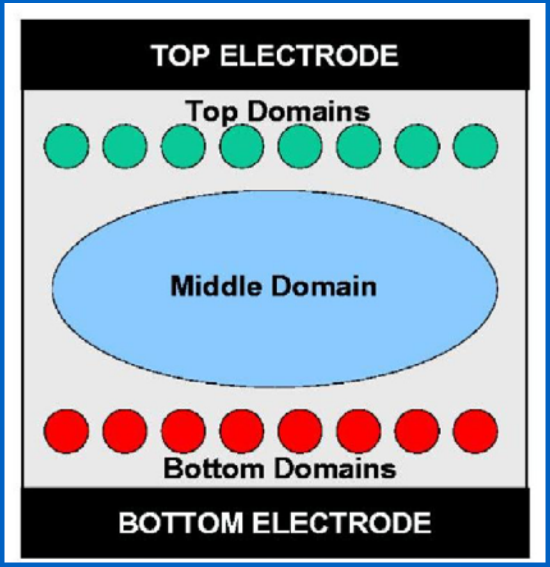



**Relation with quantum Criticality and Heavy Fermions? (Vlad D.'s talk)**

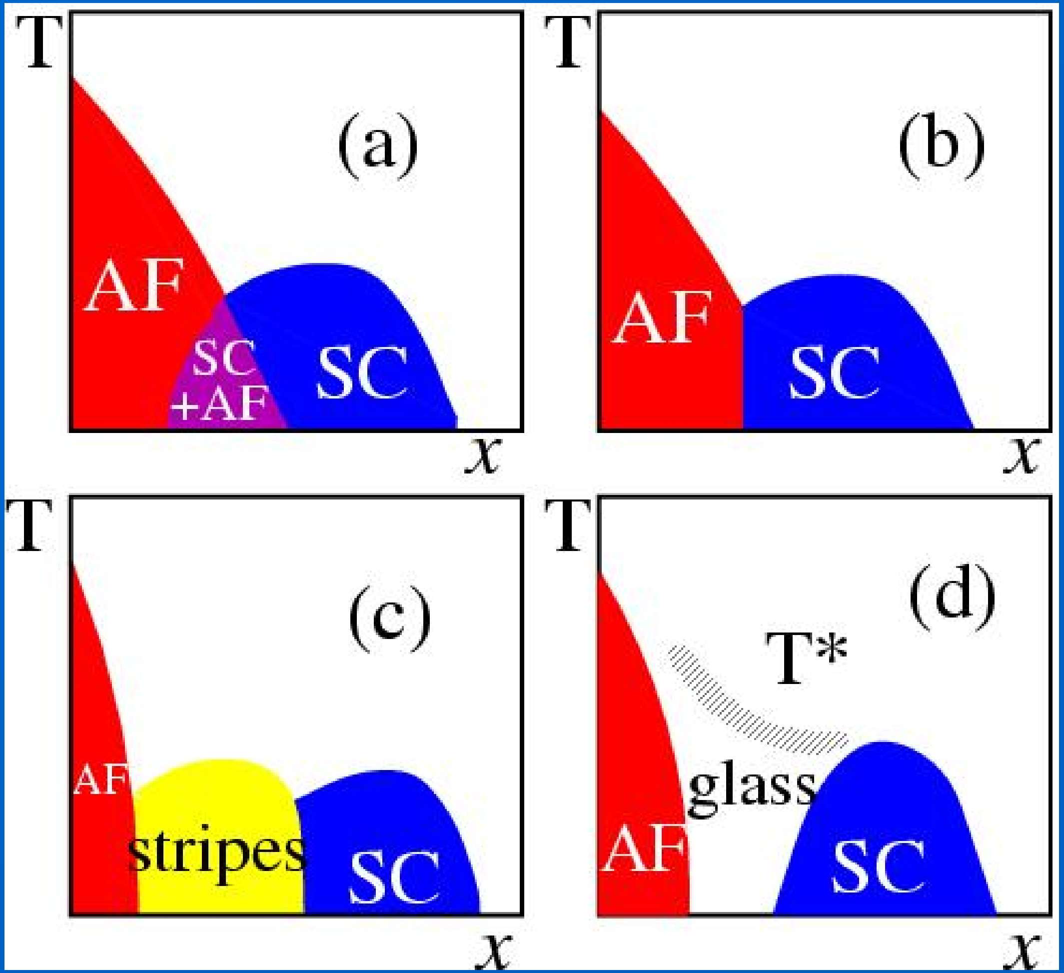
# Functionality from Complexity?



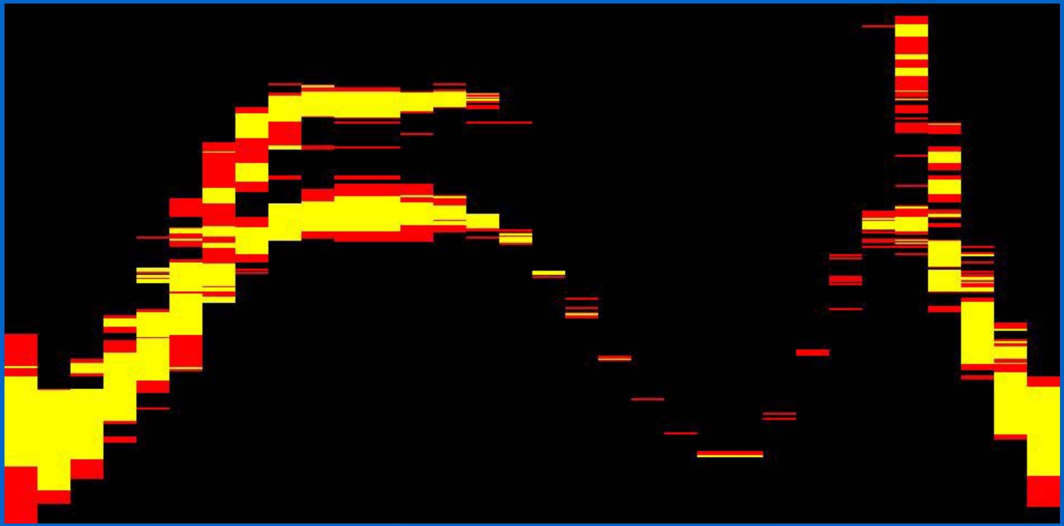



# New proposal for high-Tc: Possibilities for the AF-SC competition

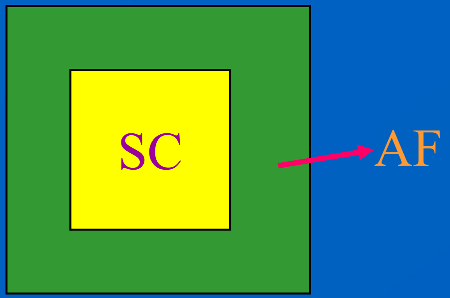


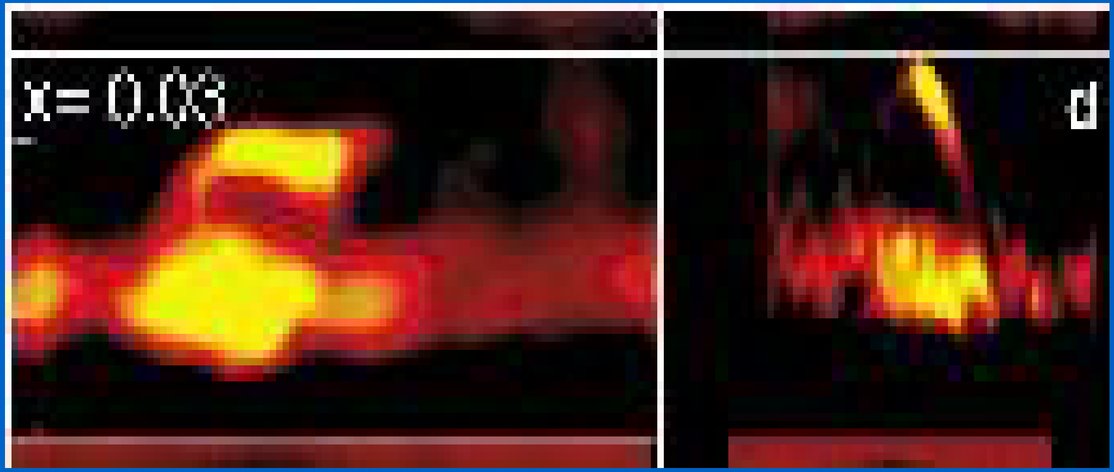

Other possibility:
SC+AF+CDW
may be competing!

# Theory vs Experiment
## (M. Mayr et al., preprint)



Quasiparticle dispersion in 20x20 cluster 60% AF and 40% d-wave SC.
Alvarez et al.

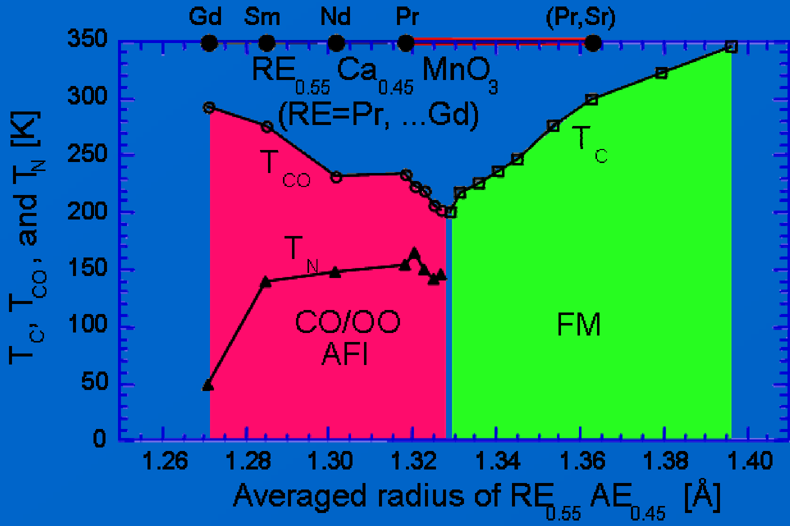


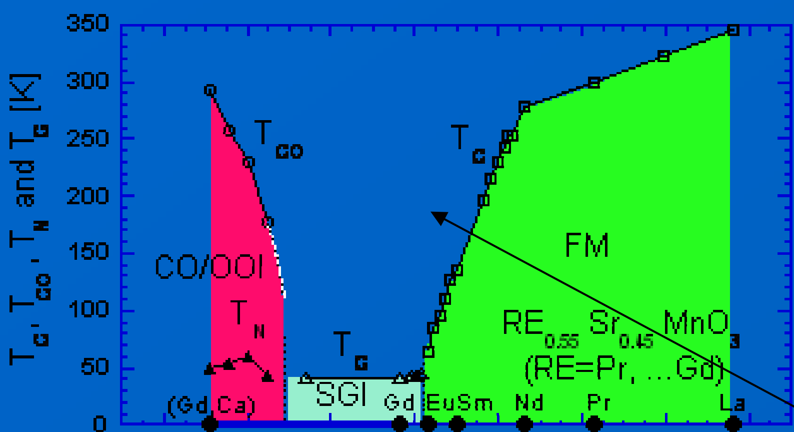



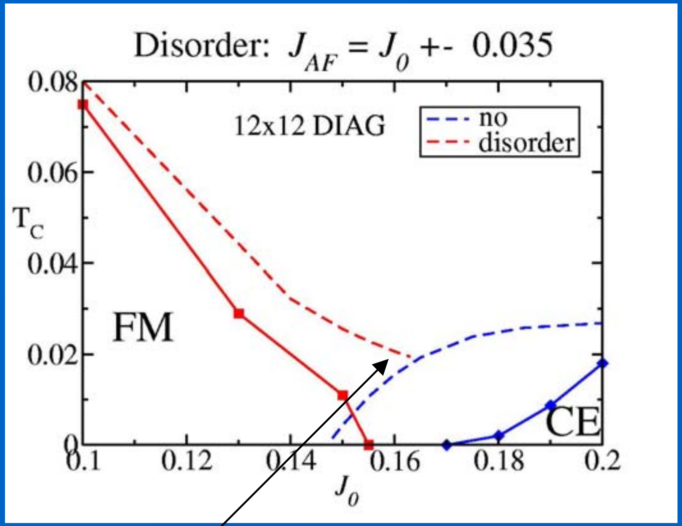

Spin Glass region (no SC)

ARPES
Yoshida, Fujimori, et al. PRL

# Recent results in agreement with overall picture




Sergienko et al., unpublished.
Two-band DE model.

Region of ``giant'' responses (softness)

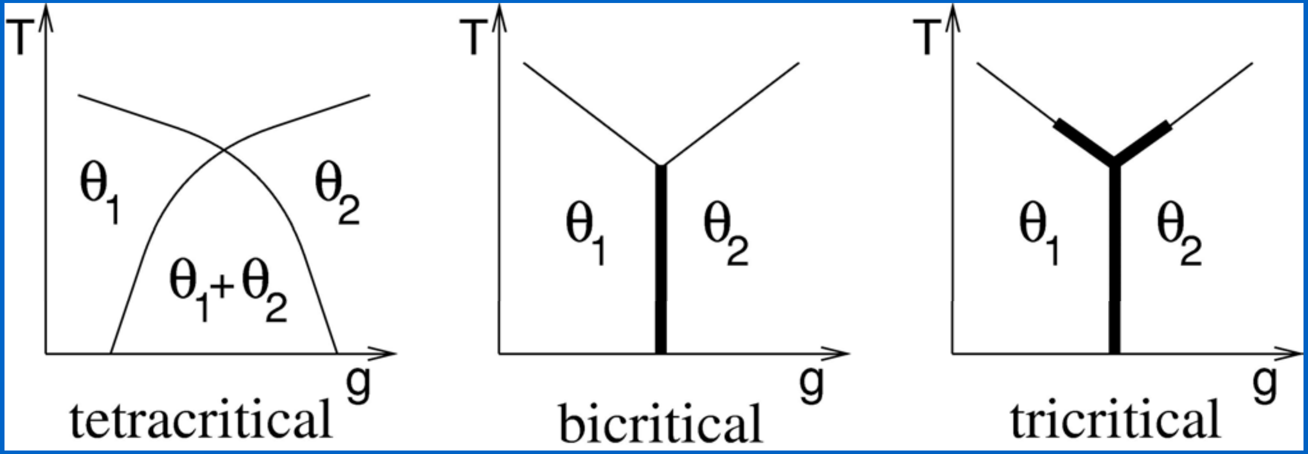
Tomioka and Tokura, PRB70, 014432 (2004)

# Recent trends suggest complexity in hard materials, such as transition-metal oxides

- **``Complex systems exist on the *edge of chaos* – they may exhibit almost regular behavior, but also can change dramatically and stochastically in time and/or space as a result of small changes in conditions.''**

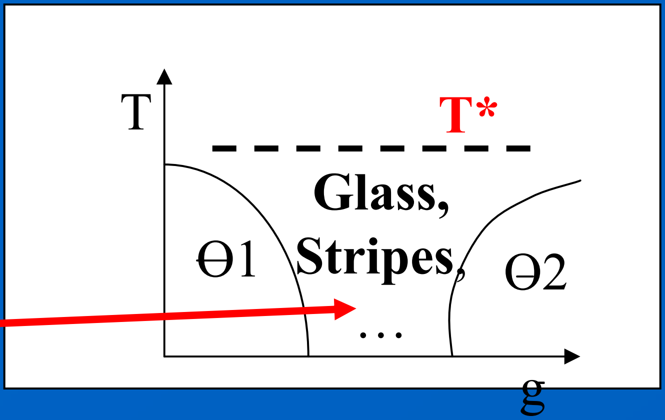
T. Vicsek, Nature 418, 131 (2002).

# Conclusions: revised menu

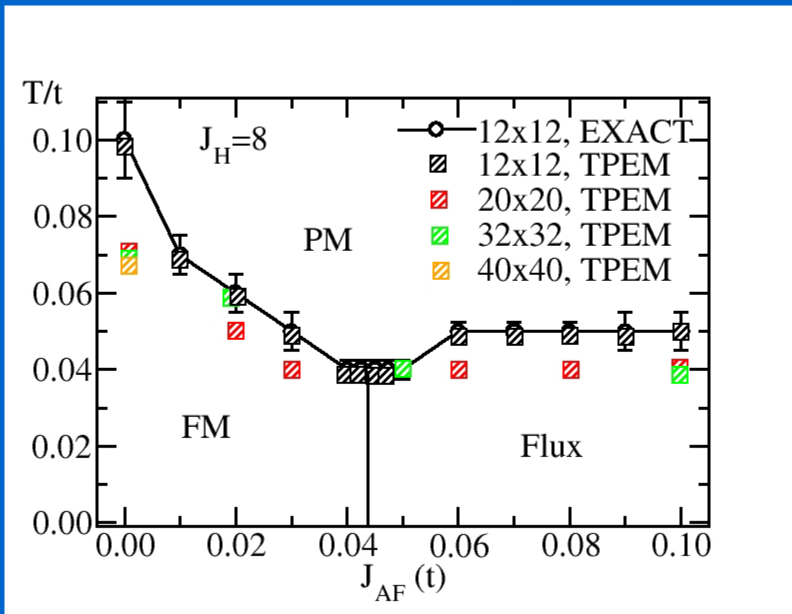


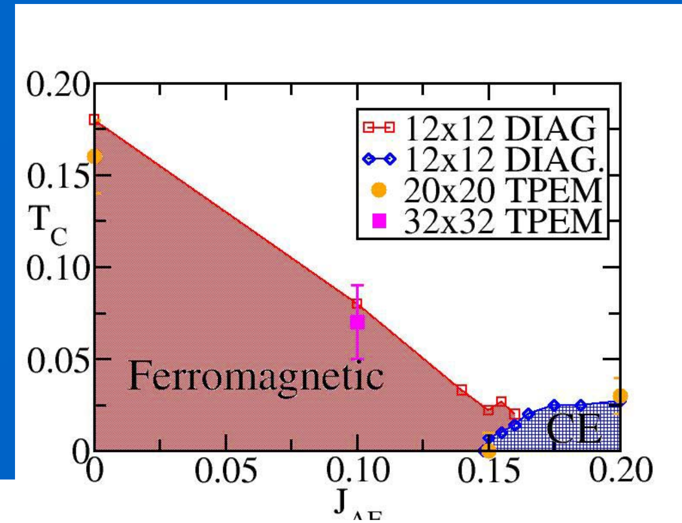

Standard

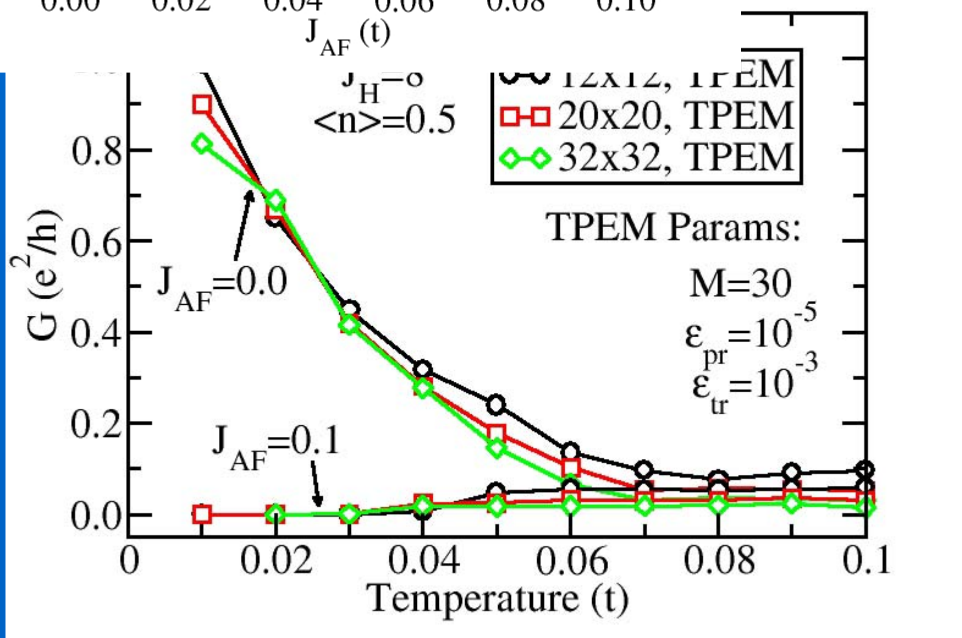
NEW

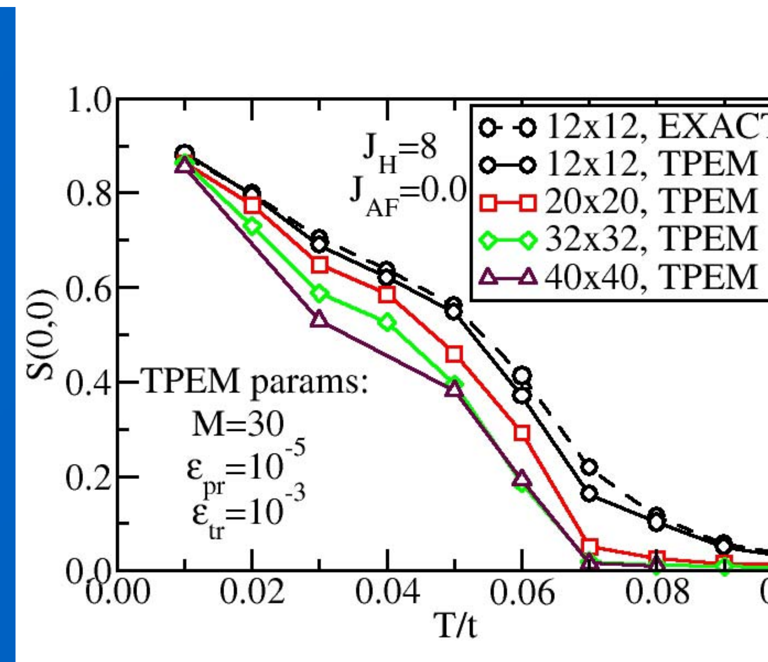



Giant effects?

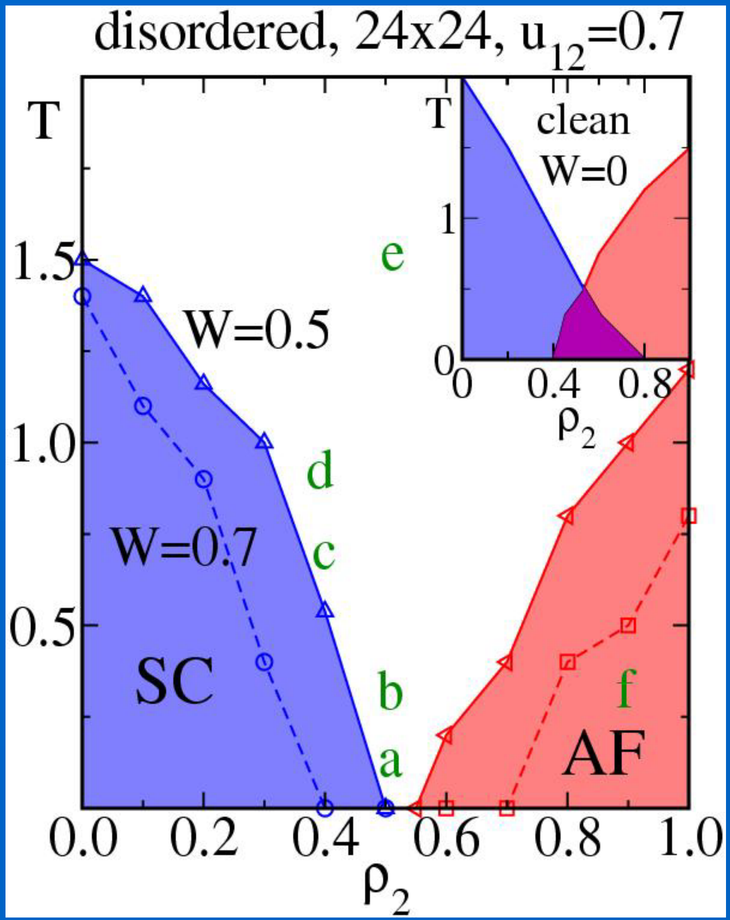

T/t
$J_H$=8
PM
FM
Flux
12x12, EXACT
12x12, TPEM
20x20, TPEM
32x32, TPEM
40x40, TPEM
0.00
0.02
0.04
0.06
0.08
0.10
$J_{AF}$ (t)

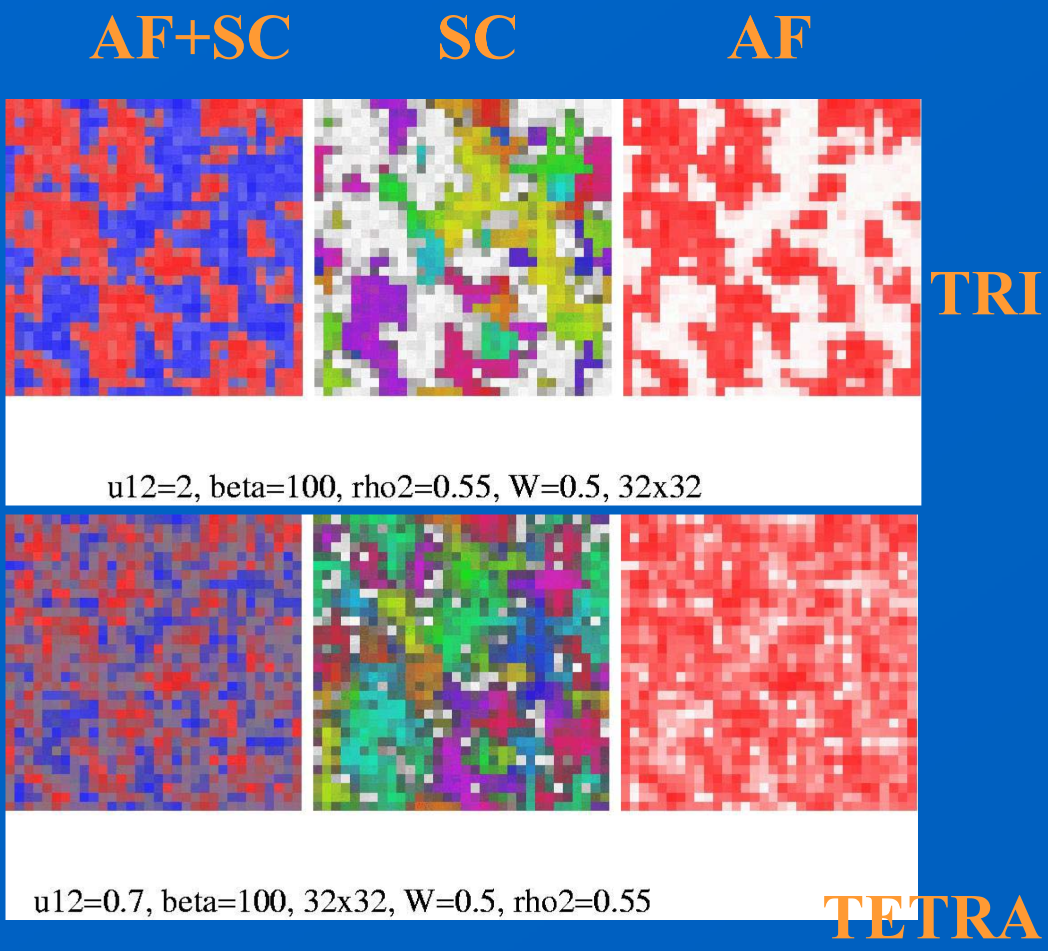

$T_C$
Ferromagnetic
CE
12x12 DIAG
12x12 DIAG.
20x20 TPEM
32x32 TPEM
0
0.05
0.10
0.15
0.20


$J_H$=8
<n>=0.5
12x12, TPEM
20x20, TPEM
32x32, TPEM
TPEM Params:
M=30
$\varepsilon_{pr}=10^{-5}$
$\varepsilon_{tr}=10^{-3}$
$J_{AF}$=0.0
$J_{AF}$=0.1
G ($e^2$/h)
0.0
0.2
0.4
0.6
0.8
0
0.02
0.04
0.06
0.08
0.1
Temperature (t)

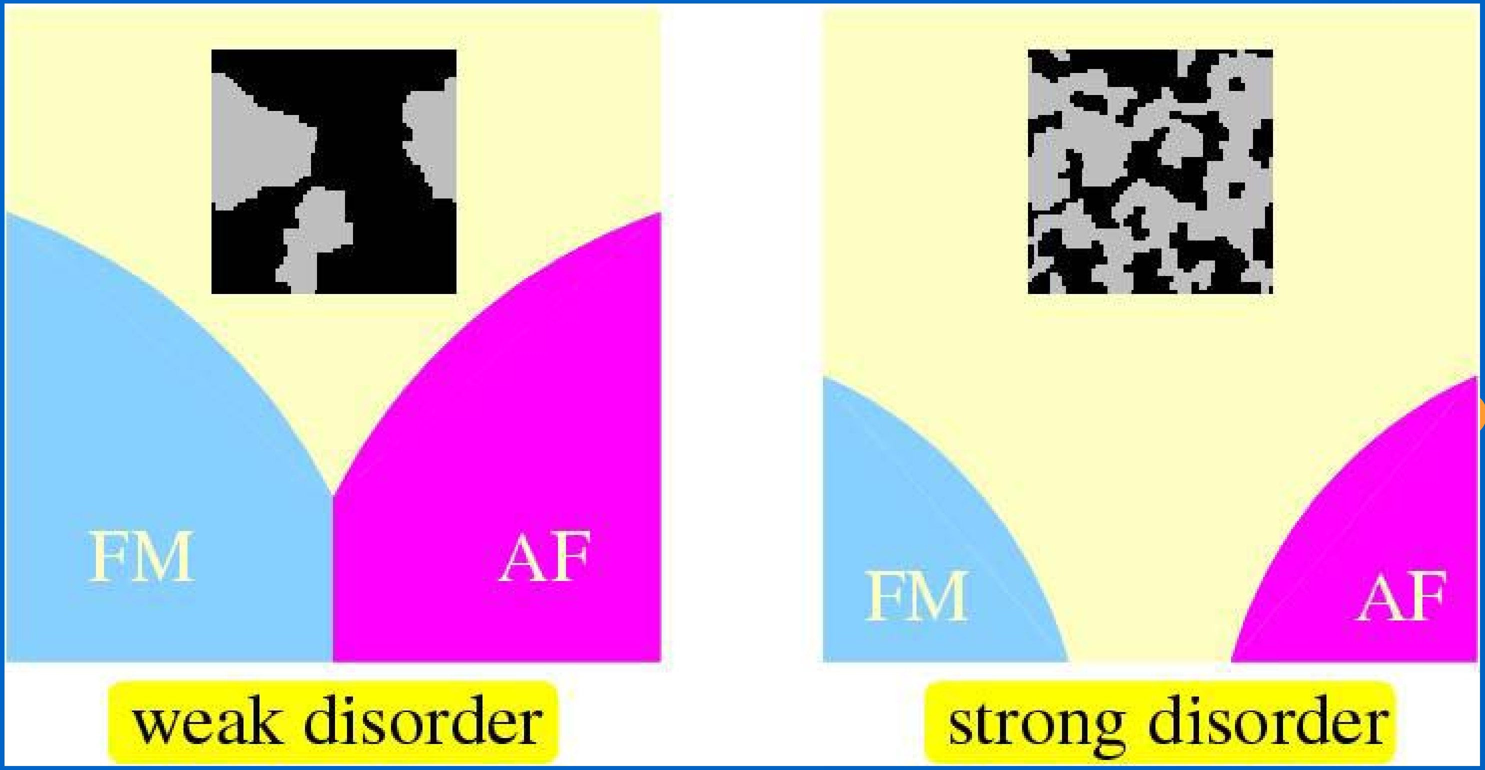

$J_H$=8
$J_{AF}$=0.0
12x12, EXACT
12x12, TPEM
20x20, TPEM
32x32, TPEM
40x40, TPEM
TPEM params:
M=30
$\varepsilon_{pr}=10^{-5}$
$\varepsilon_{tr}=10^{-3}$
S(0,0)
0.0
0.2
0.4
0.6
0.8
1.0
0.00
0.02
0.04
0.06
0.08
T/t

# Effects of Quenched Disorder on a model with only AF and SC order parameters (no mobile electrons).



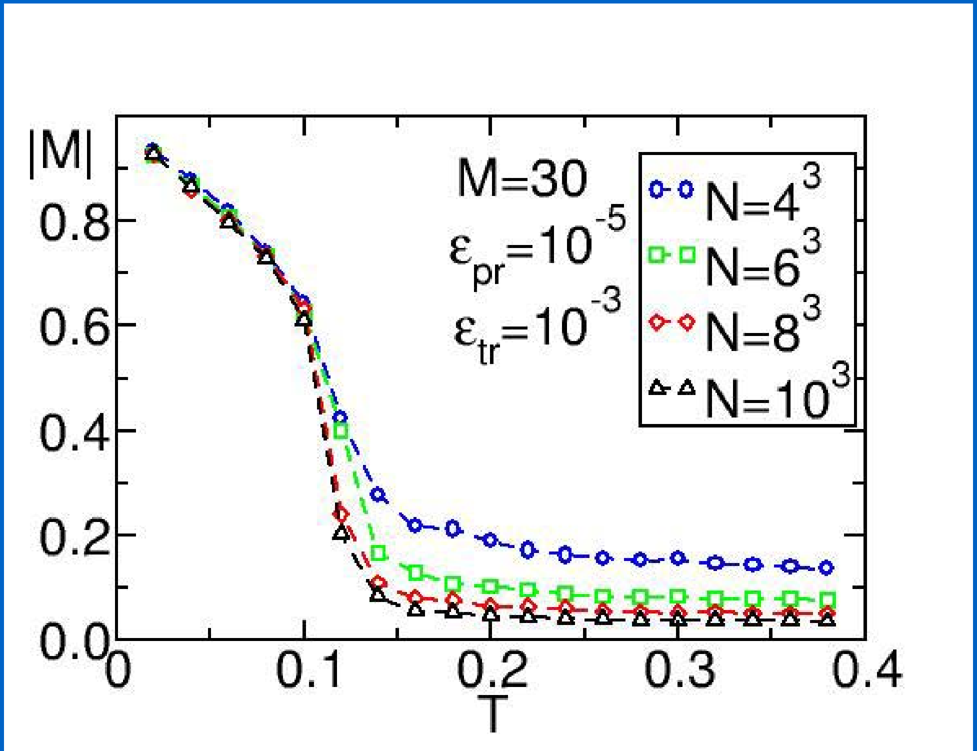



# Cluster size?




Clusters sizes are not universal. They depend on disorder strength, unless long-range interactions are introduced.

# New algorithms (Motome et al., Aliaga): 1000 sites can be easily reached

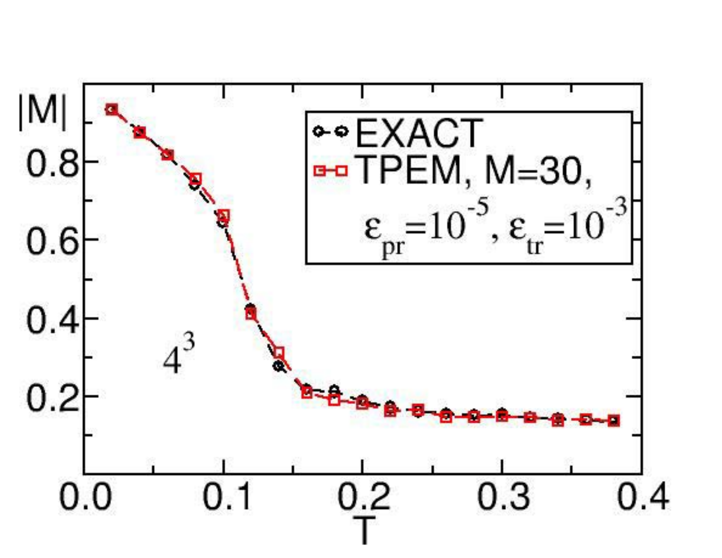


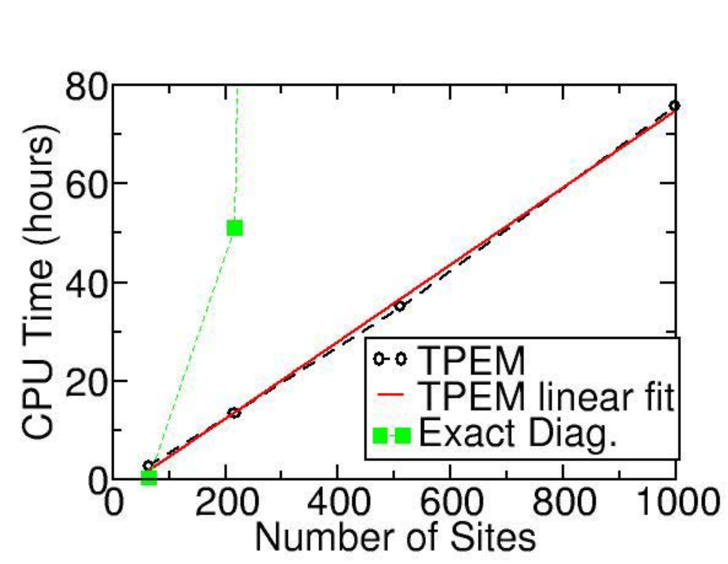

At least in two dimensions the study of percolation with DE models may happen soon (36x36 clusters).

# New algorithms under development

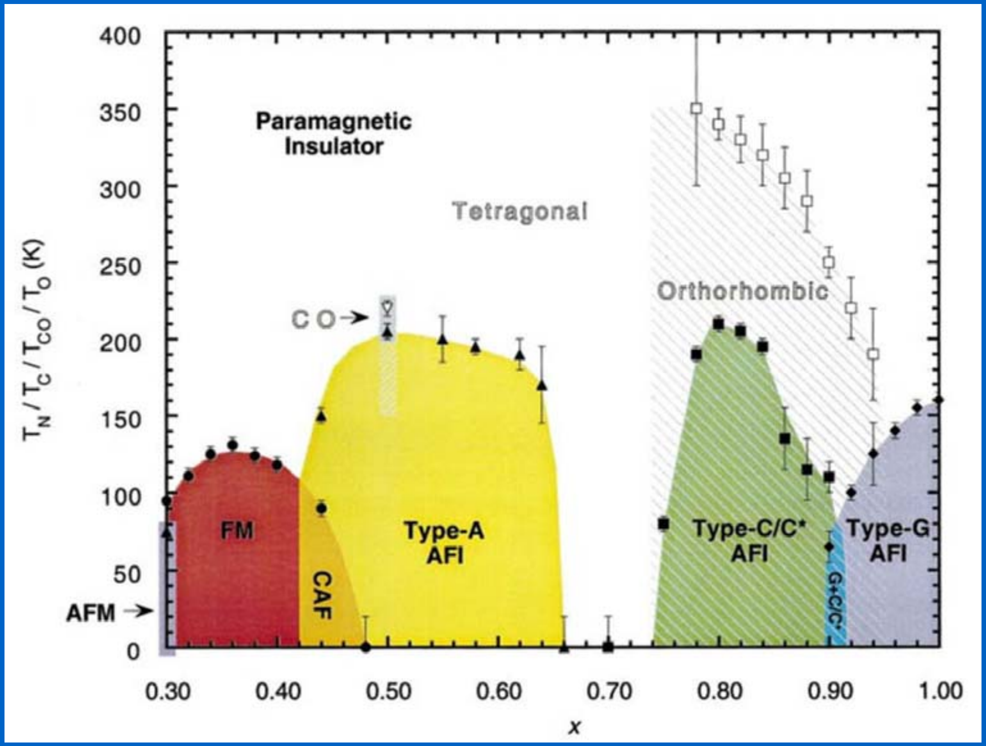
Current technique scales as $N^4$.   Strong limitations in 3D. CMR only observed in ``toy models'' thus far.

New method (Furukawa et al.) is of order N. Focus on DOS, obtained via a Chebyshev polynomial expansion. Works in localized electron basis, uses local nature of MC updates, and sparse Hamiltonian.



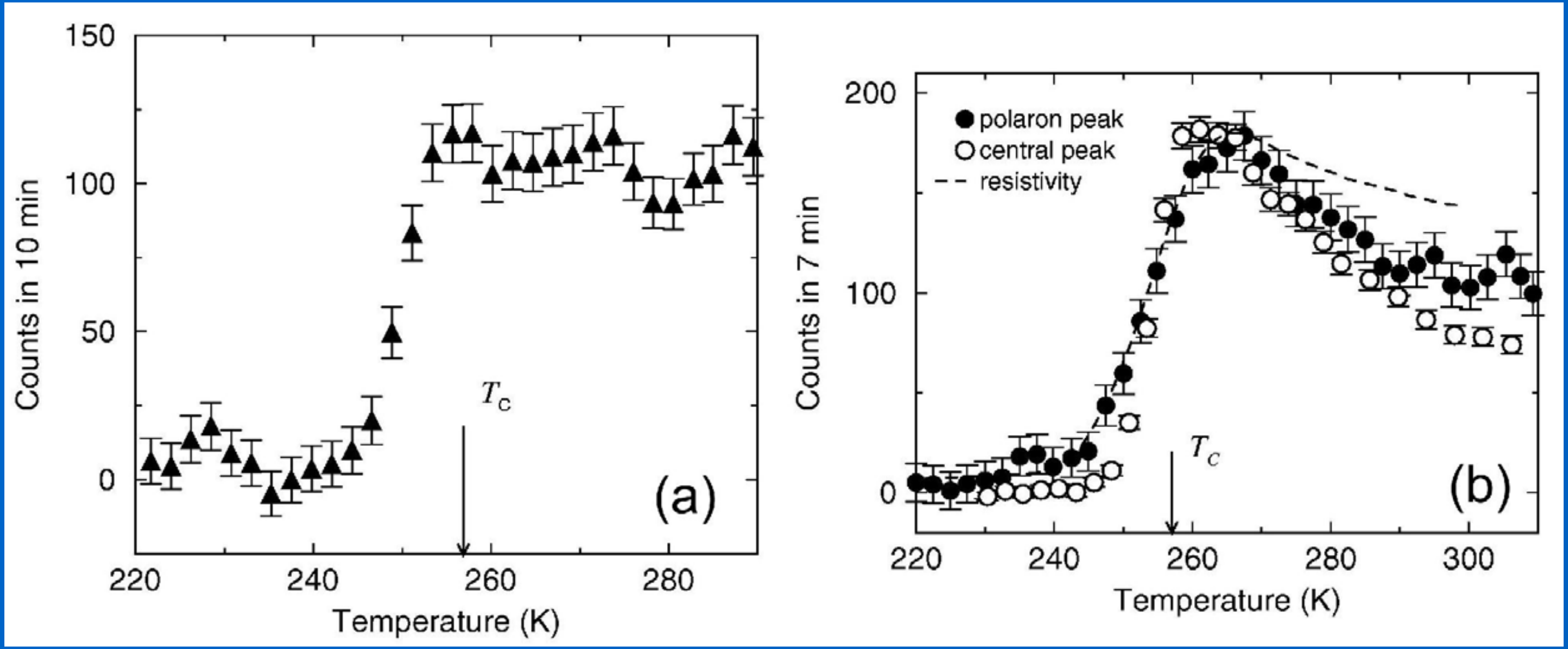



# Bilayer Phase Diagram




J. Mitchell et al.

# ``Correlated polarons''
# (a.k.a. short-range charge order) above Tc

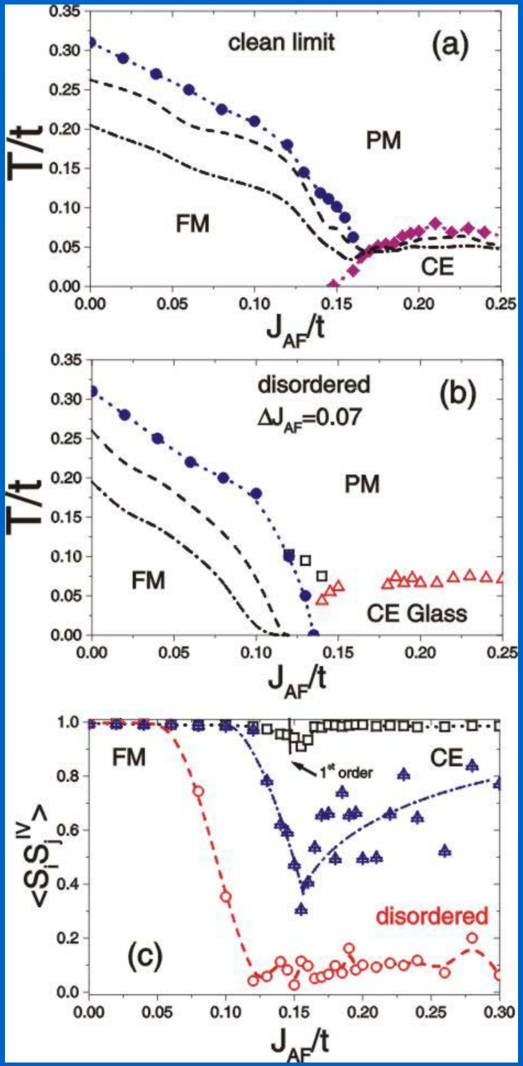



Uncorrelated polarons
Nearly T-independent

Correlated polarons
Follows resistivity vs. T

Results from Adams et al, PRL.. See also
P. Dai et al., PRL, D. Argyriou et al.. PRL, and others.

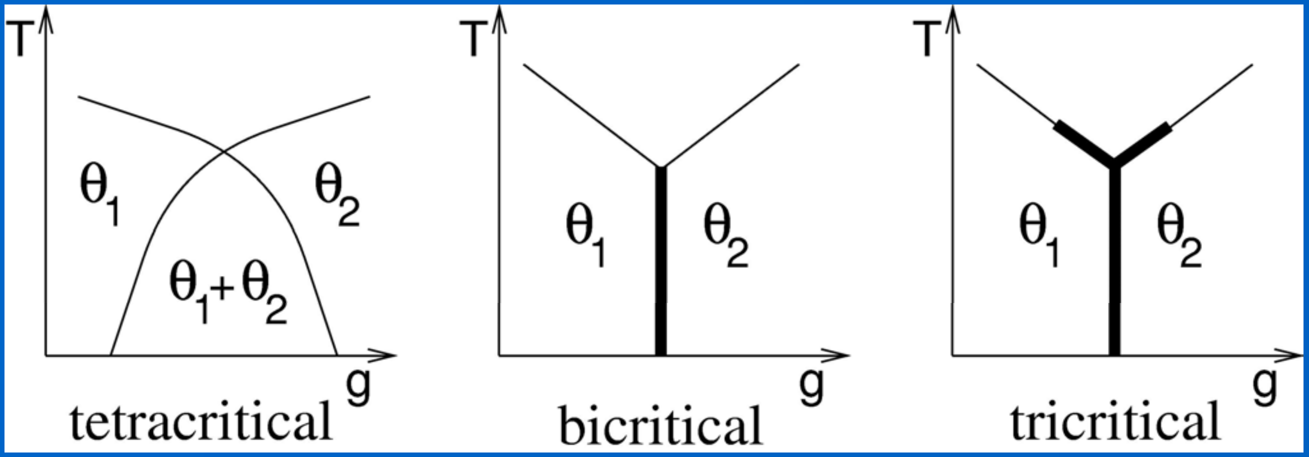
# New: CE-phase is sensitive to disorder




X=0.5

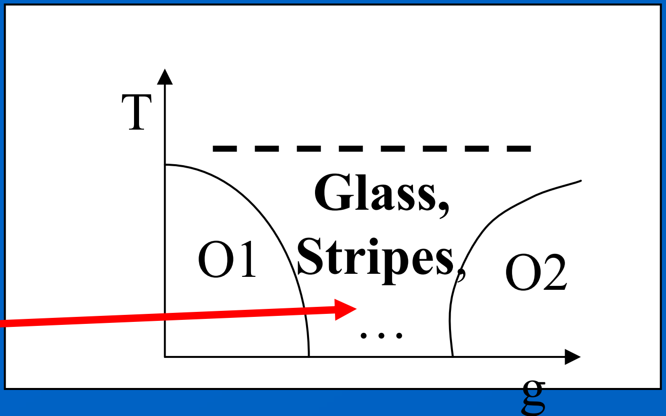
FM-AF transition is first-order and ``bicritical'' looking. Disorder affects the CE phase strongly, similarly as in experiments (Aliaga et al., preprint)

# Conclusions: revised menu

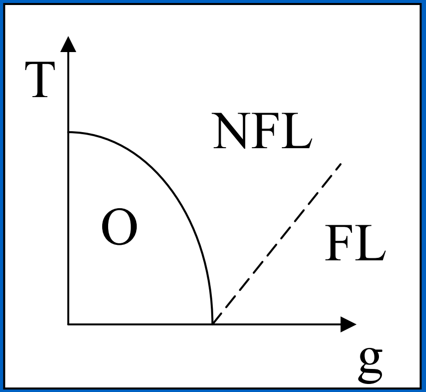



**OLD LG**

**NEW**

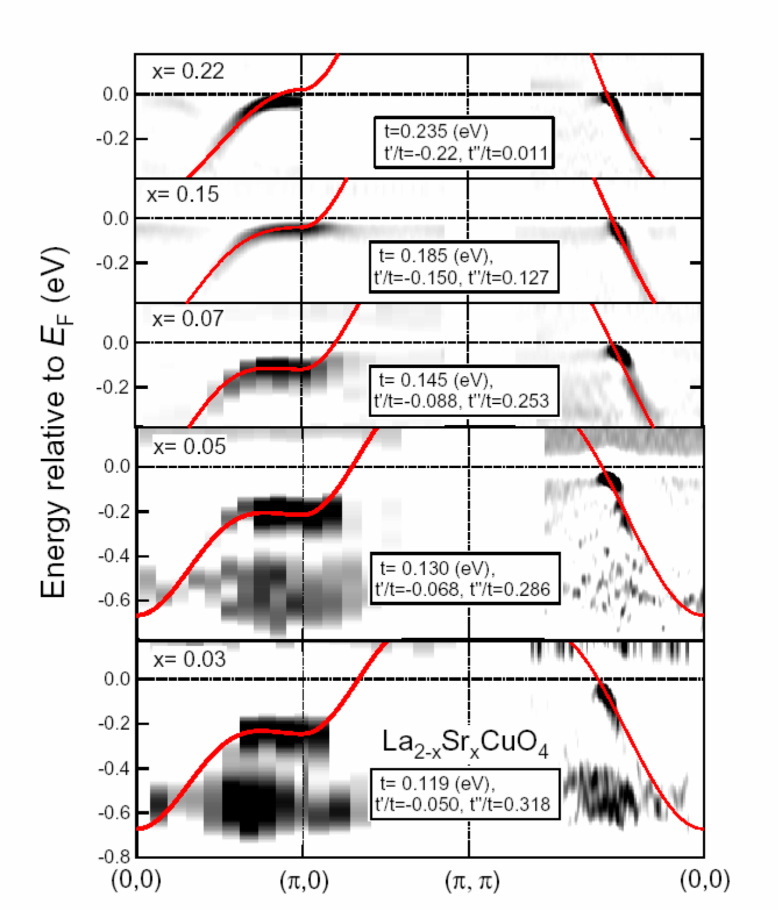



**Giant effects?**

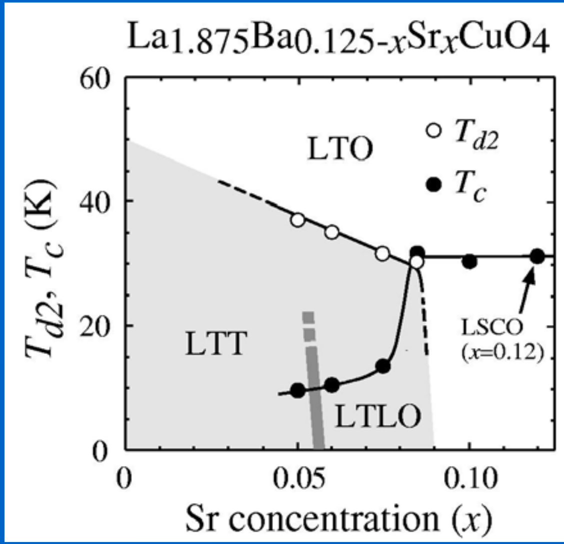



**Relation with quantum criticality?**

# First-order transitions in cuprates? Are stripes universal?




Fujimori et al.

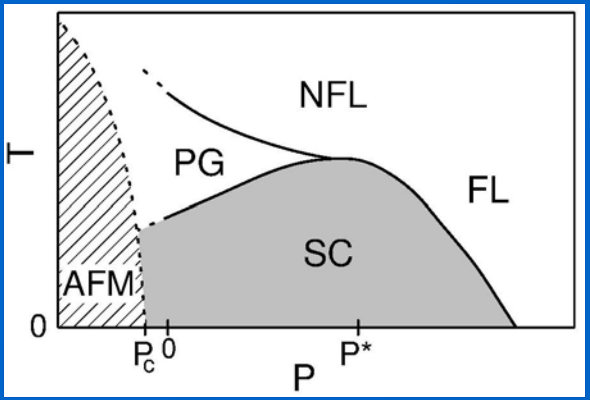


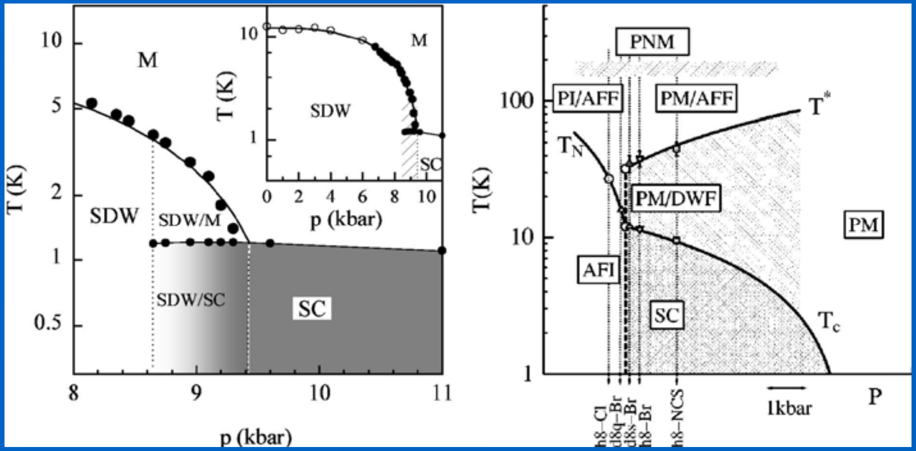

Fujita et al.
Elastic N. Scatt.

**See also electron doped Cu-oxides, organic SC.**

**_ Not a**
**have s**

# Heavy Fermions and Organic SC have similar features

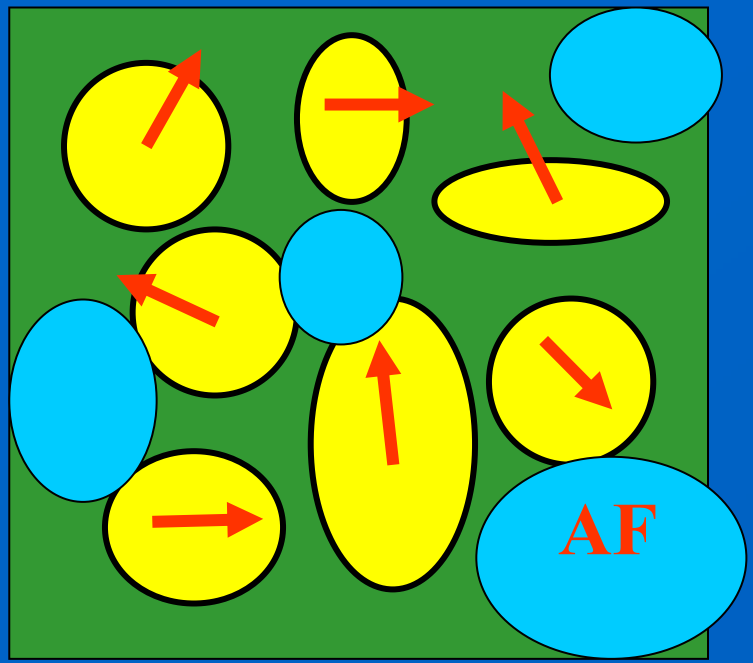



Ce-based heavy fermion
(Los Alamos)

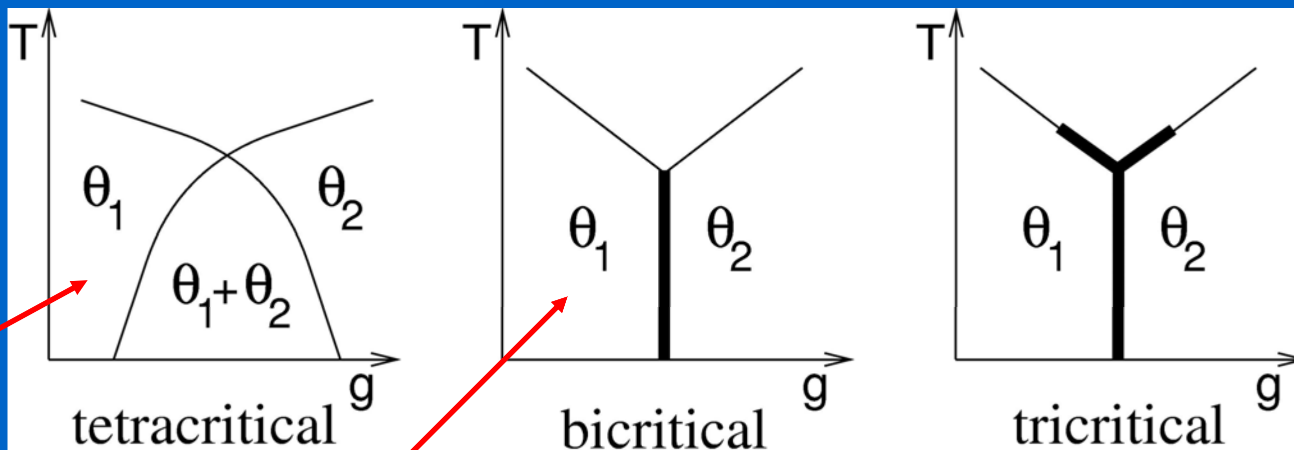
Organic superconductors:
SDW/SC coexistence or
First-order SC-SDW transition

# Cartoonish summary
(Alvarez et al., cond-mat/0401474)



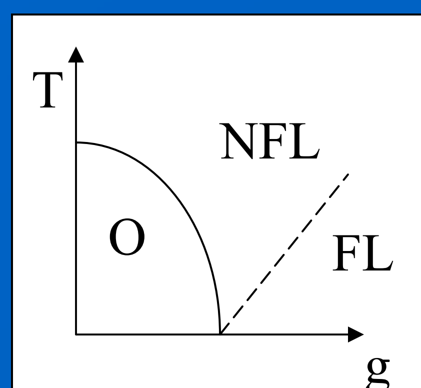

**Proposed: Random orientation of the local SC phase in glassy underdoped region**

# Bi-tri-tetra critical



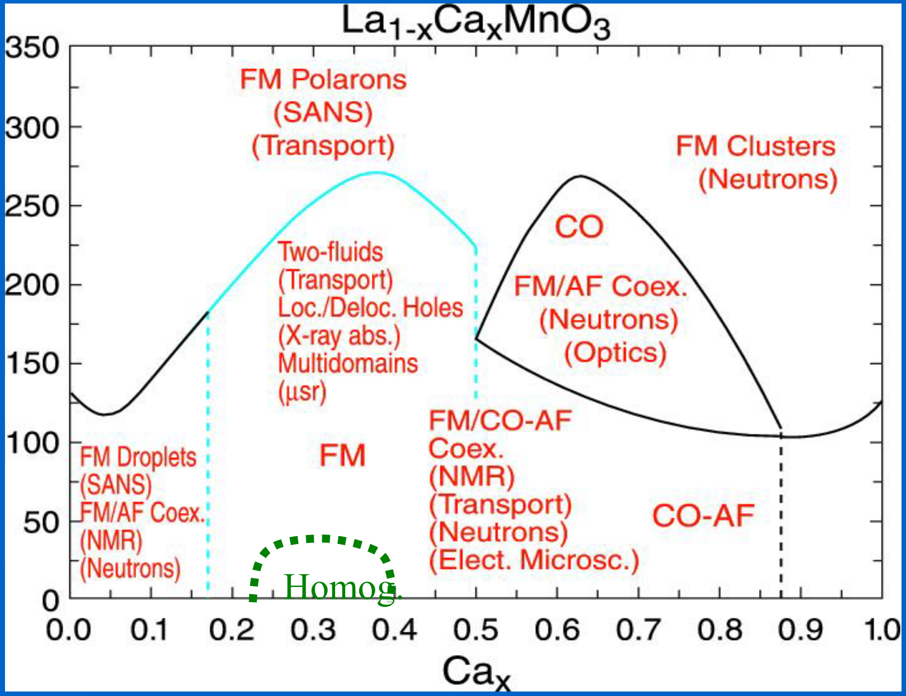

$u_{12} < 1$

$u_{12} \geq 1$

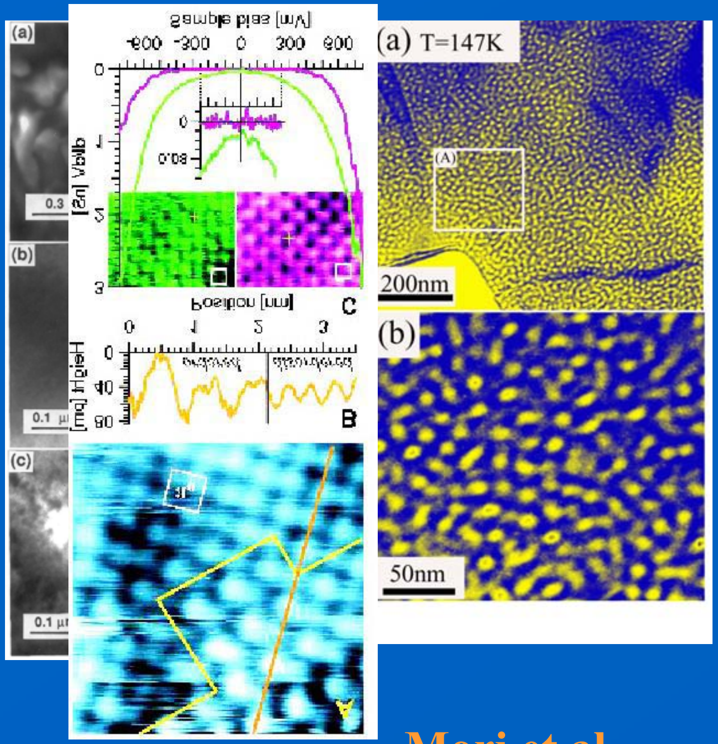



**Relation with quantum criticality?**

# Recent Trends: Phase Coexistence in Manganites




A.Moreo et al.,
Science 283, 2034 (1999).




**Uehara et al., Nature '99 LaPrCaMnO EM**

Renner et al., Nature '02 BiCaMnO STM

**Mori et al. Lorentz micros.**

**FM nanodomains**

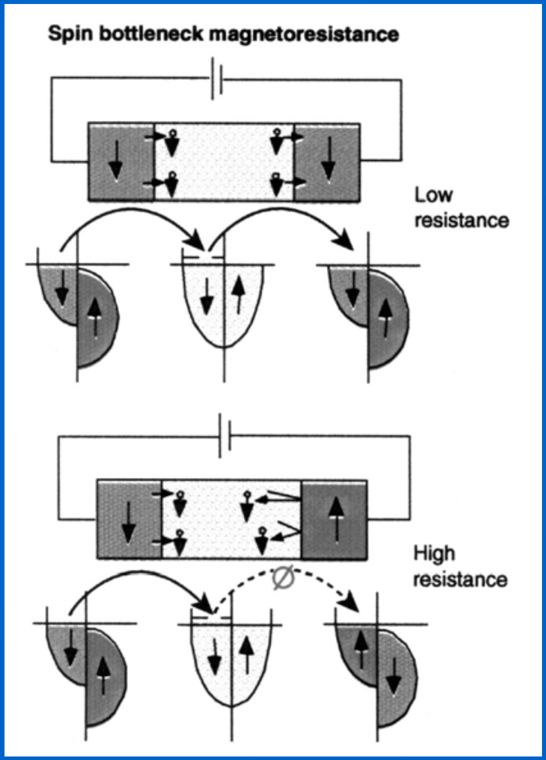
**Tc=85K, T*=170K**

$La_{0.25}Pr_{0.375}Ca_{0.375}MnO_3$

**… plus many many other important papers!**

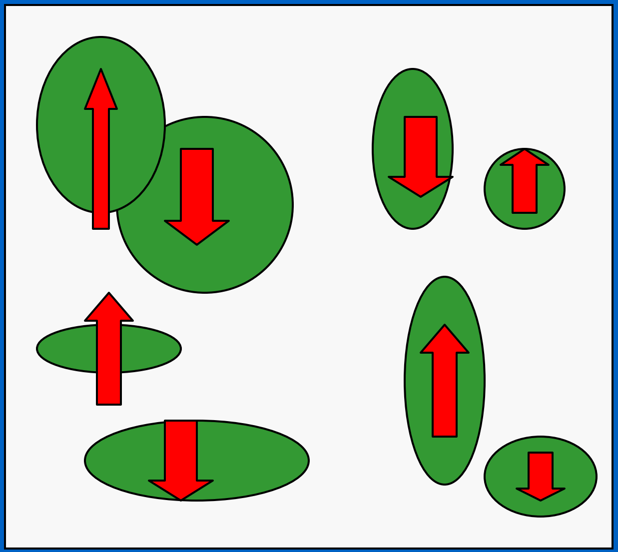
# Similarities with GMR effect ?

GMR




Prinz

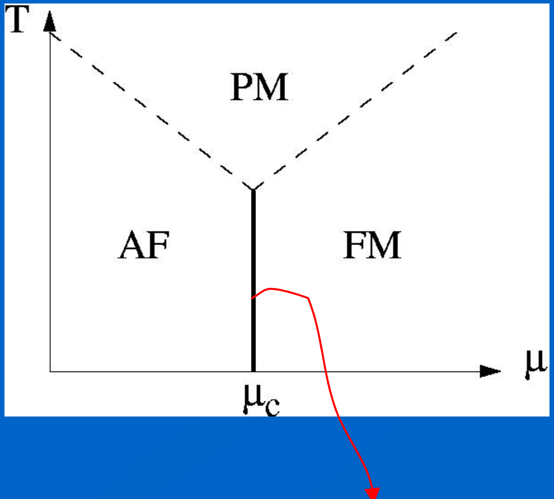
CMR



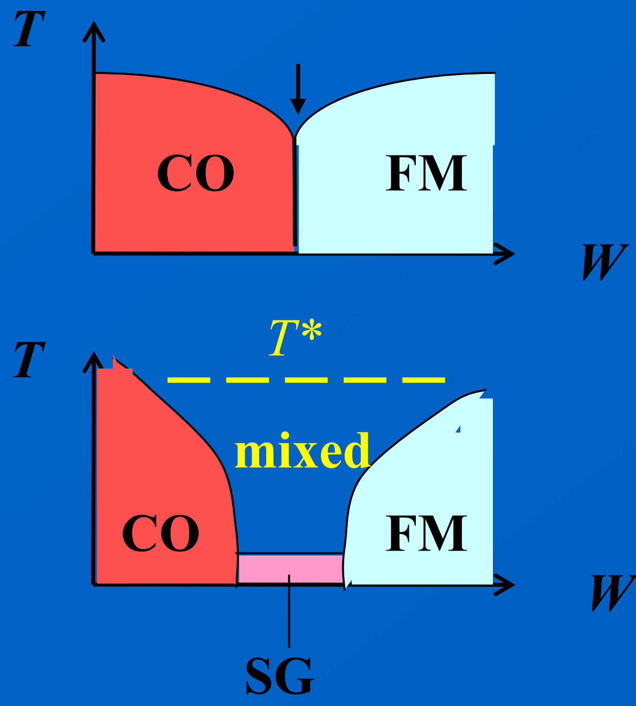
GMR at small distances?

# Phase Competition in the Presence of Quenched Disorder

Clean limit




First order

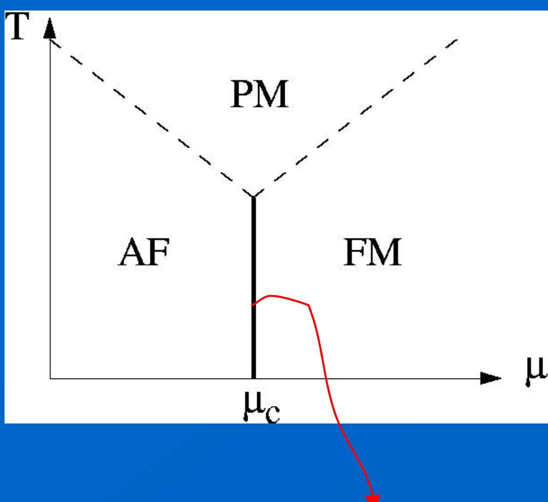



Toy Model with Disorder Burgy et al., PRL87, 277202 (2001). See also Nagaosa et al. T* also discussed by Salamon.

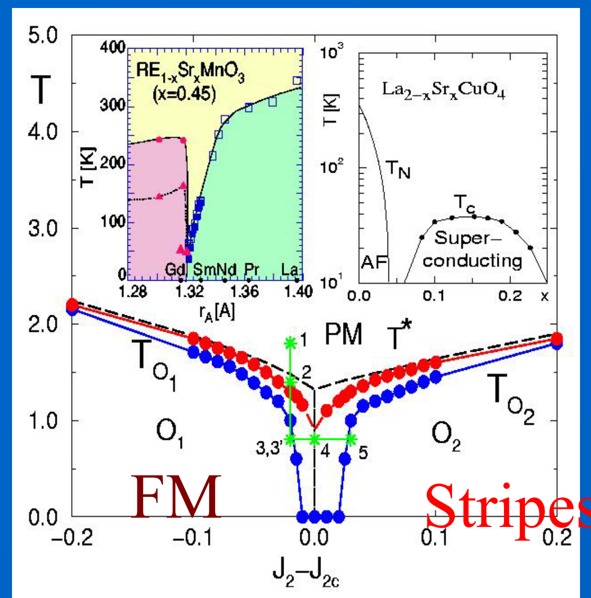
For experiments see Akahoshi et al. PRL 2003; Argyriou et al., PRL; De Teresa

# Phase Competition in the Presence of Quenched Disorder

Clean limit result:



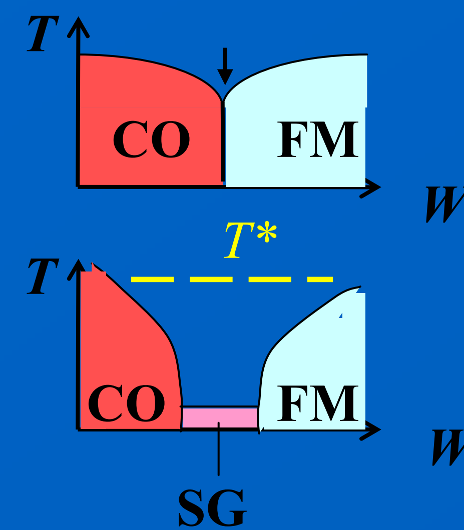

First order




Toy Model with disorder

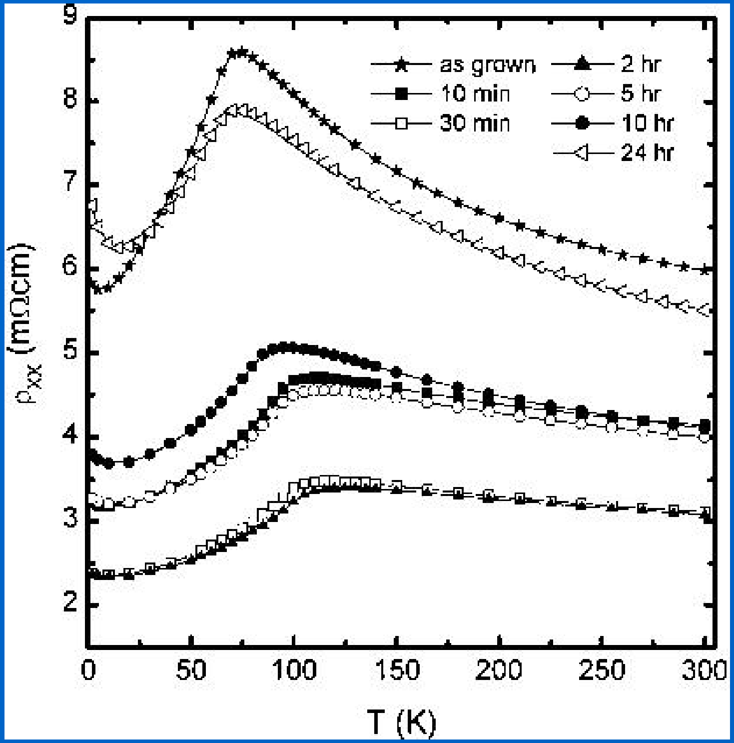
Burgy et al., PRL87, 277202 (2001).

See also Nagaosa et al.



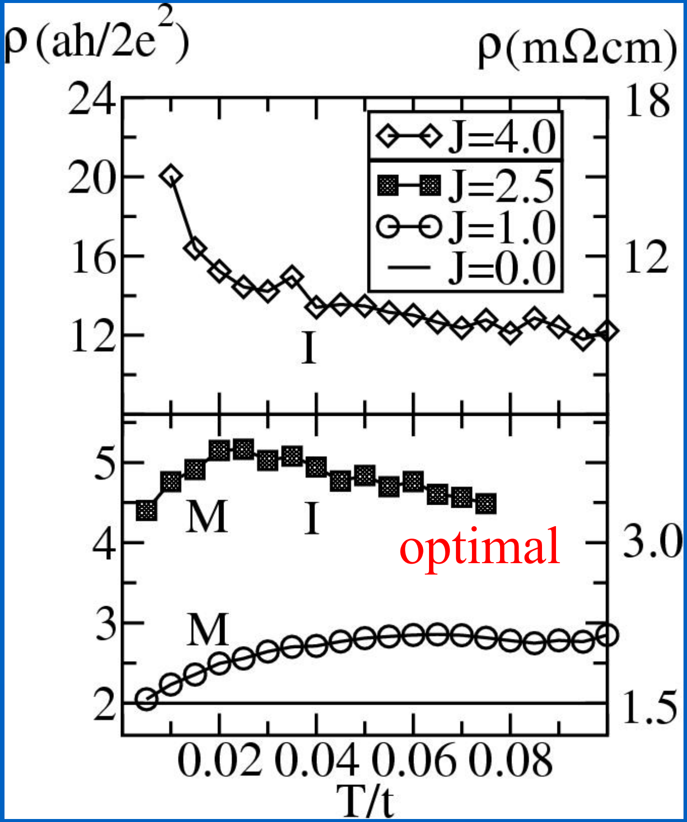

See also Akahoshi et al. PRL 2003; Argyriou et al., PRL; De Teresa

# Resistivity: experiments vs. theory




Penn State data

Similarities with Mn-oxides!.

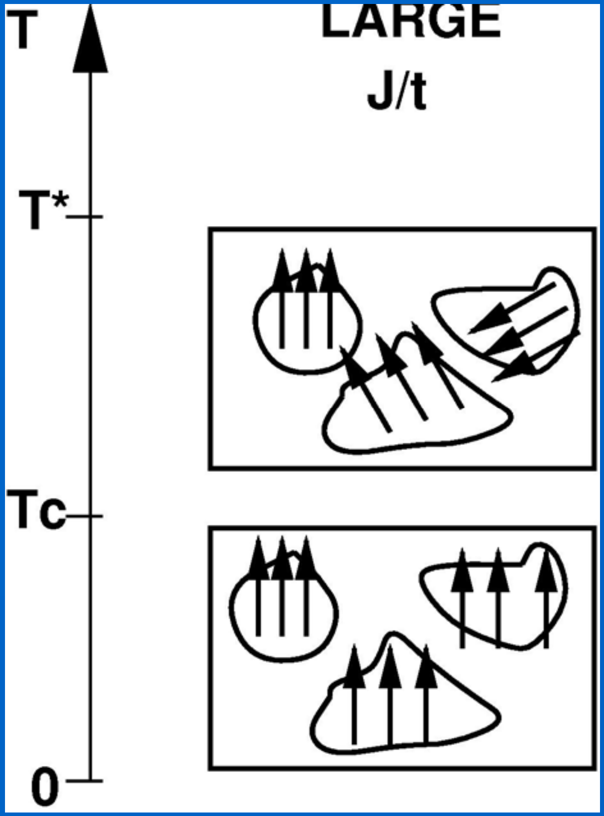



Alvarez et al., cond-mat

Technique: lead-cluster-lead

# T* in diluted magnetic semiconductors as well?

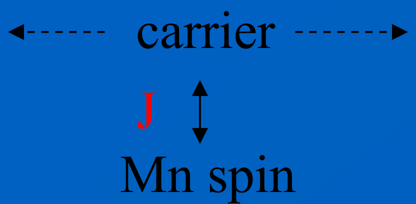
Mn-doped GaAs; x=0.1;Tc = 110K. Spintronics? Model: carriers interacting with randomly distributed Mn-spins locally




Monte Carlo simulations very similar to those for manganites.

Clustered state, insulating

FM state, metallic




Alvarez et al., PRL 89, 277202 (02). See also Mayr et al., PRB 2002

# Landau-Ginzburg effective theory

**Microscopic Theory** $(c^+c, c^+c^+cc)$

$\downarrow$

**Mean Field approximation** $\left(c^+c, \Delta^* cc, \Delta c^+c^+\right)$

$\downarrow$

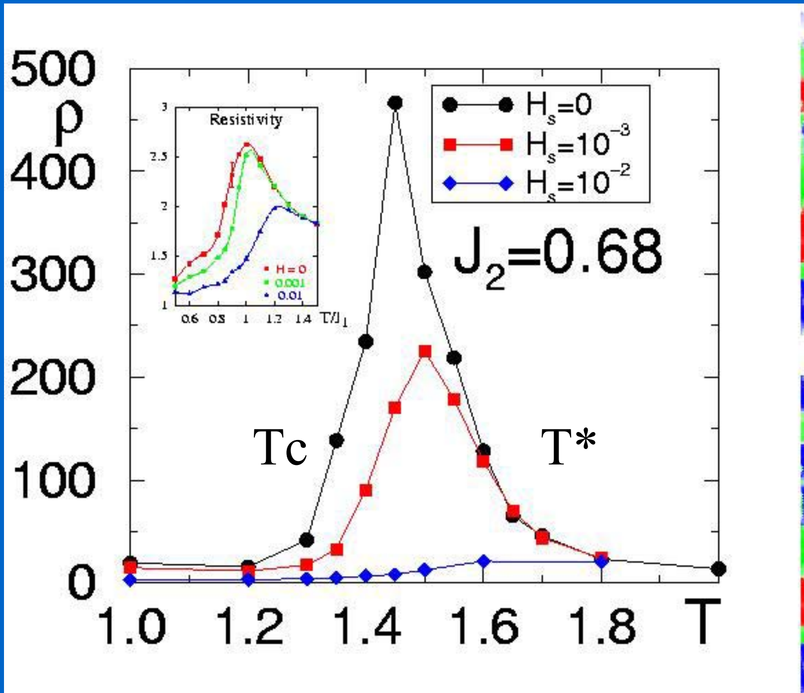
**Integrate out electrons** $(H_{eff}(\Delta, \Delta^+))$

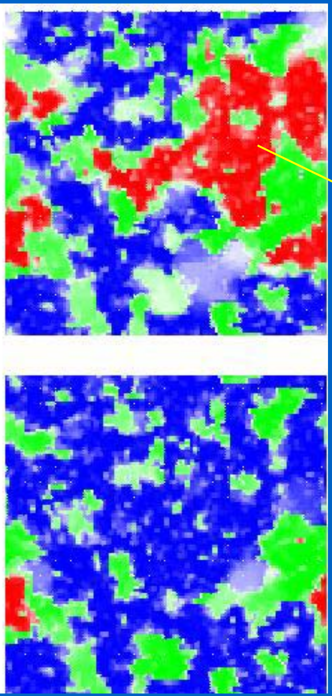
$\downarrow$

**Expand in powers of** $\Delta\ (H_{GL})$

**$H_{GL}$ can be guessed based on symmetry considerations and minimal couplings.**

# CMR effect in inhomogeneous states



H=0

Rotates easily

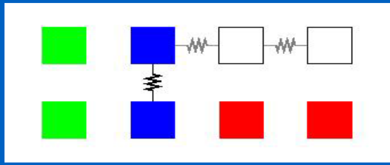
H=0.01

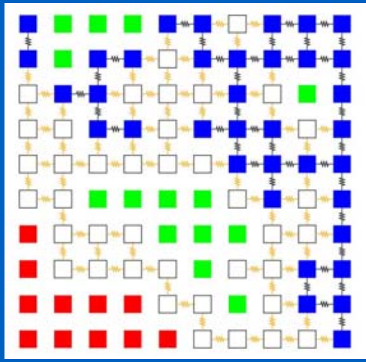
Field is small, but effective spin is large!

MR ratios as large as 1000% at H=0.01.

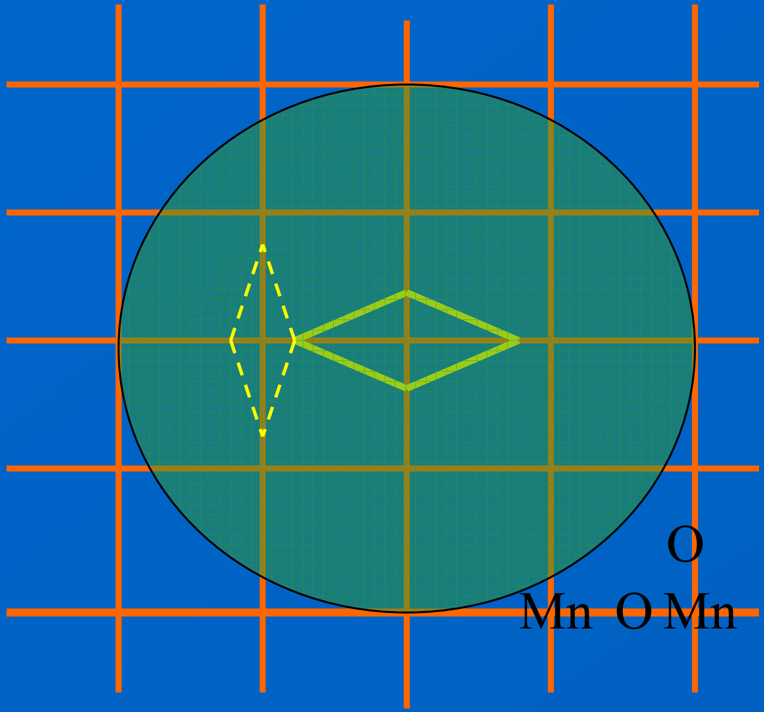
Resistor Network:

FM up FM down Insulator Disorder





# Relevance of Correlated Disorder




Cooperative JT distortions create correlations, i.e. distortions propagate

Elastic effects generate $1/r^3$ power-law correlations.

# “Landau-Ginzburg” effective model

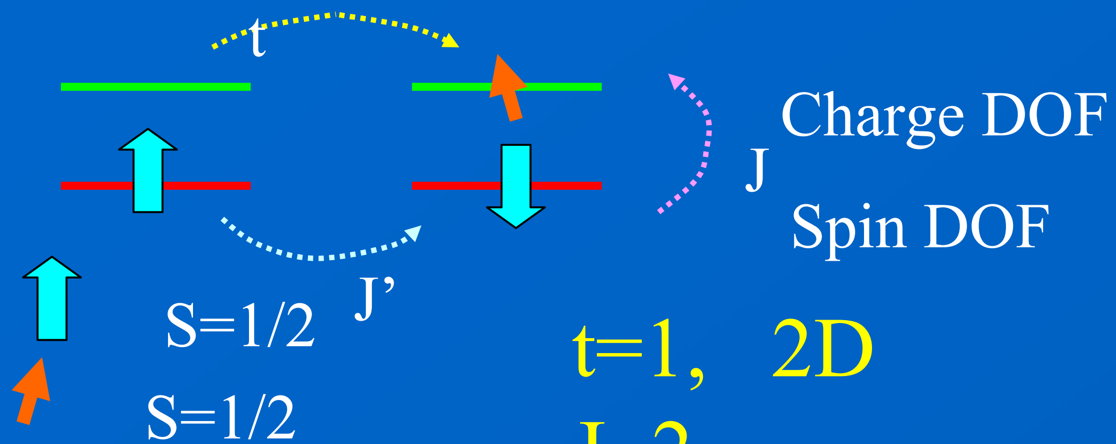
$$H = r_1 \sum_i |\Delta_i|^2 + \frac{u_1}{2} \sum_i |\Delta_i|^4 + \rho_1 \sum_{<i,j>} |\Delta_i||\Delta_j| \cos(\Psi_i - \Psi_j) +$$

$$r_2 \sum_i |S_i|^2 + \frac{u_2}{2} \sum_i |S_i|^4 + \rho_2 \sum_{<i,j>} \vec{S}_i . \vec{S}_j + u_{12} \sum_i |\Delta_i|^2 |S_i|^2$$

$$\vec{S}_i = S_i(\sin\theta_i \cos\varphi_i, \sin\theta_i \sin\varphi_i, \cos\theta_i)$$

$$\Delta_i = |\Delta_i| e^{i\psi_i}$$

# A Spin-Fermion Model as a phenomenological model for HTSC




t=1, 2D

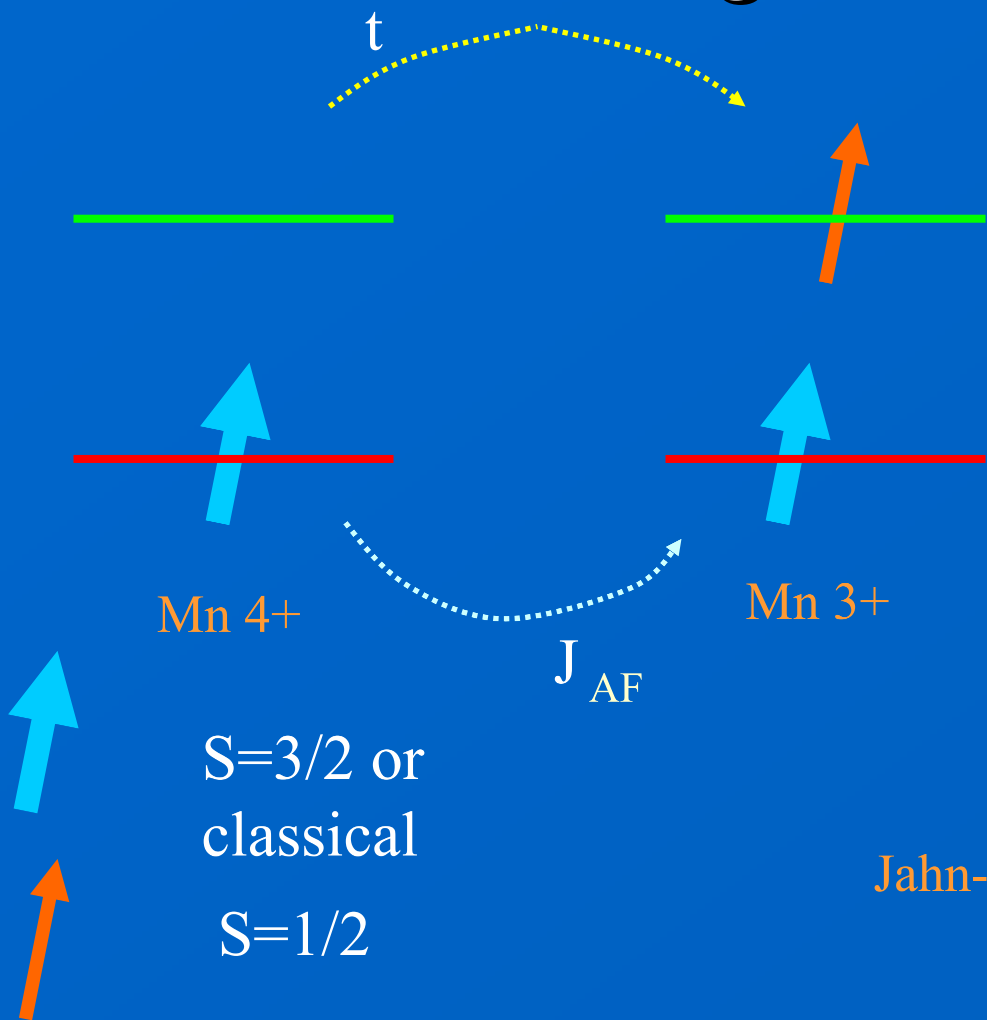
J~2

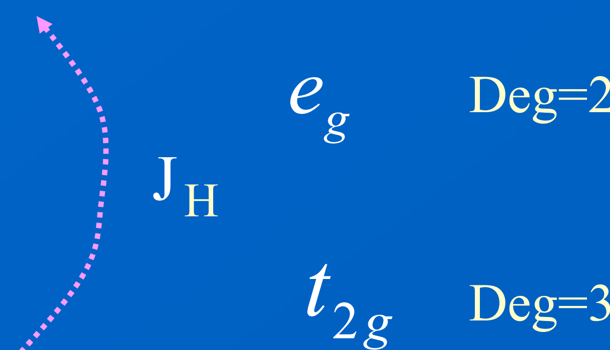
J'=0.05

$$H = -t\sum_{\langle i,j\rangle}\left(c^{+}_{i,\sigma}c_{j,\sigma} + c^{+}_{j,\sigma}c_{i,\sigma}\right) + J\sum_{i} s_i \cdot S_i + J'\sum_{\langle i,j\rangle} S_i \cdot S_j$$

Moreo et al., PRL 84, 2690 (2000); PRL 88, 187001 (2002) (S classical)

# Main couplings in models for manganites

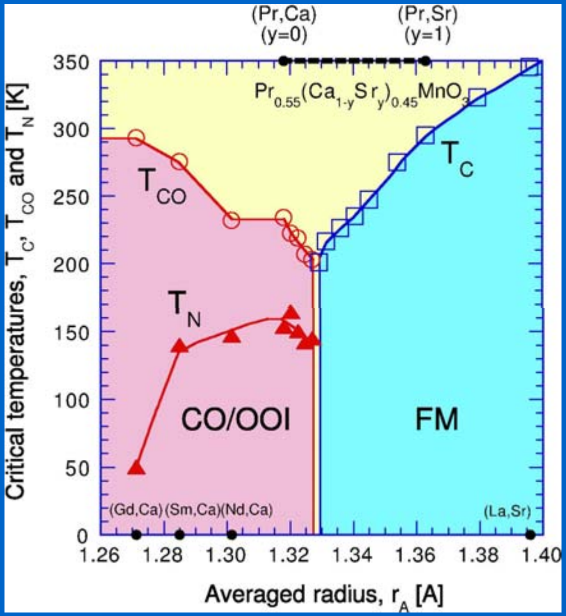



$t=1$, $J_H > 5$ (prevents double occupancy, as U does)
$J_{AF} \sim 0.1$ (small but relevant)

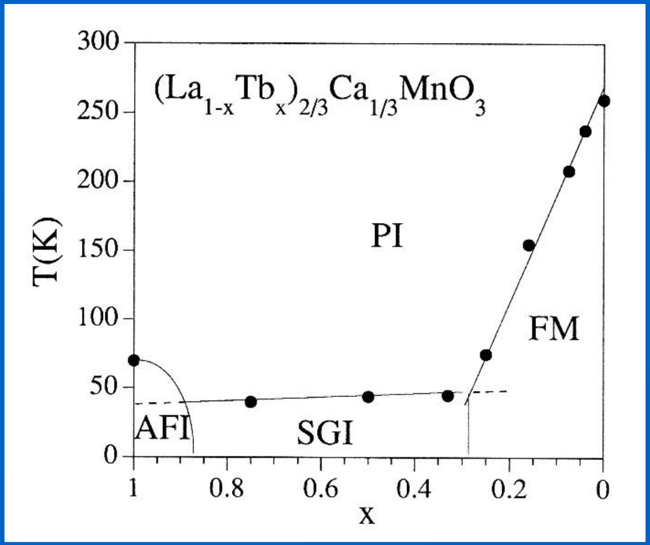
Jahn-Teller effects are also important

# Experimental Test of Predictions




"Weak" disorder

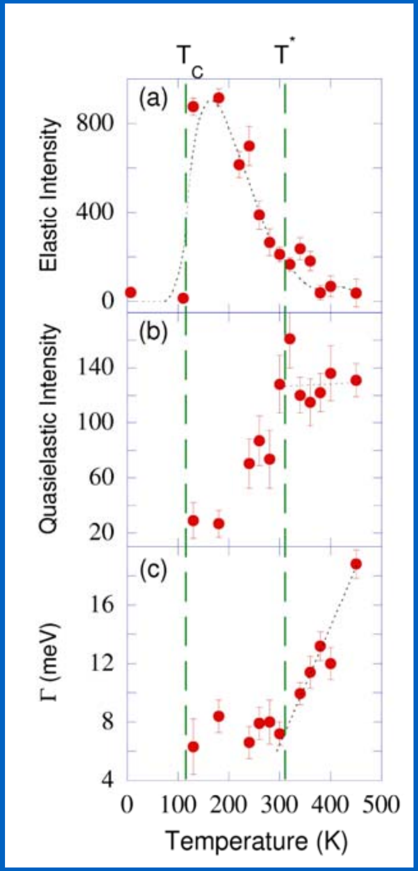
Tomioka et al.
PRB02, PRL03




"Strong" disorder

De Teresa et al.

T*>Tc

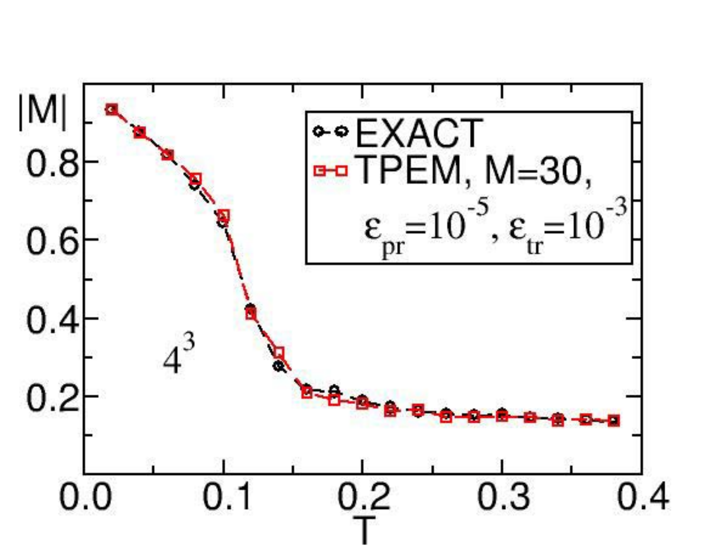


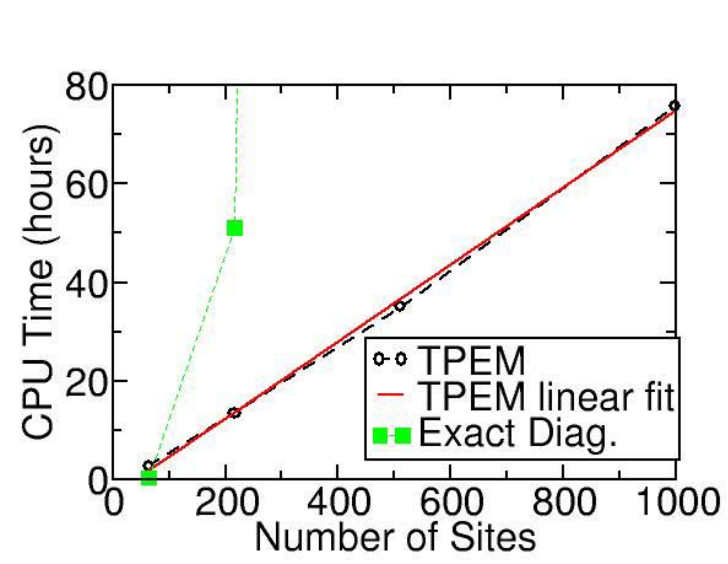

Argyriou et al. PRL

# New algorithms under development

Current technique scales as $N^4$. Strong limitations in 3D. CMR only observed in ``toy models'' thus far.

New method (Furukawa et al.) is of order N. Focus on DOS, obtained via a Chebyshev polynomial expansion. Works in localized electron basis, uses local nature of MC updates, and sparse Hamiltonian.

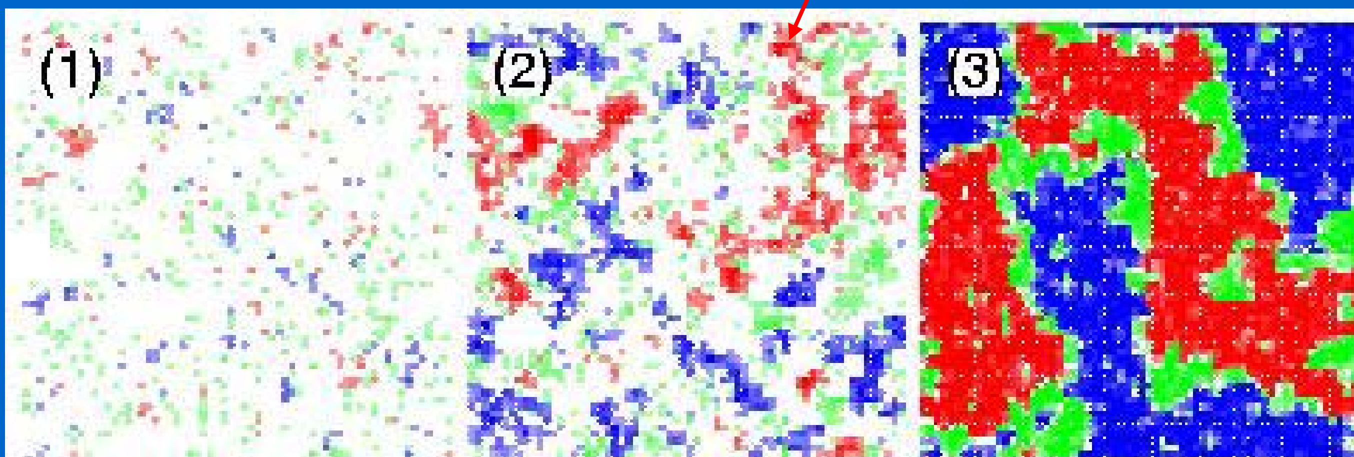


# Real-Space Spin Configurations

Quasi-static

Paramagnetic Clustered Percolated



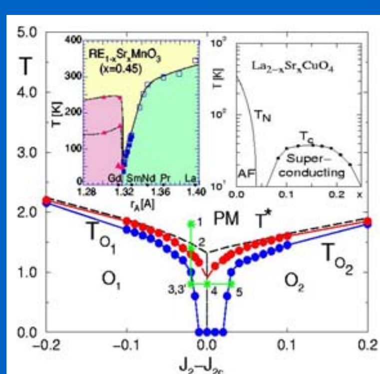

FM down
FM up
Insulator
Disorder

T>T*

$T_{o_1}<T<T^*$

$T<T_{o_1}$

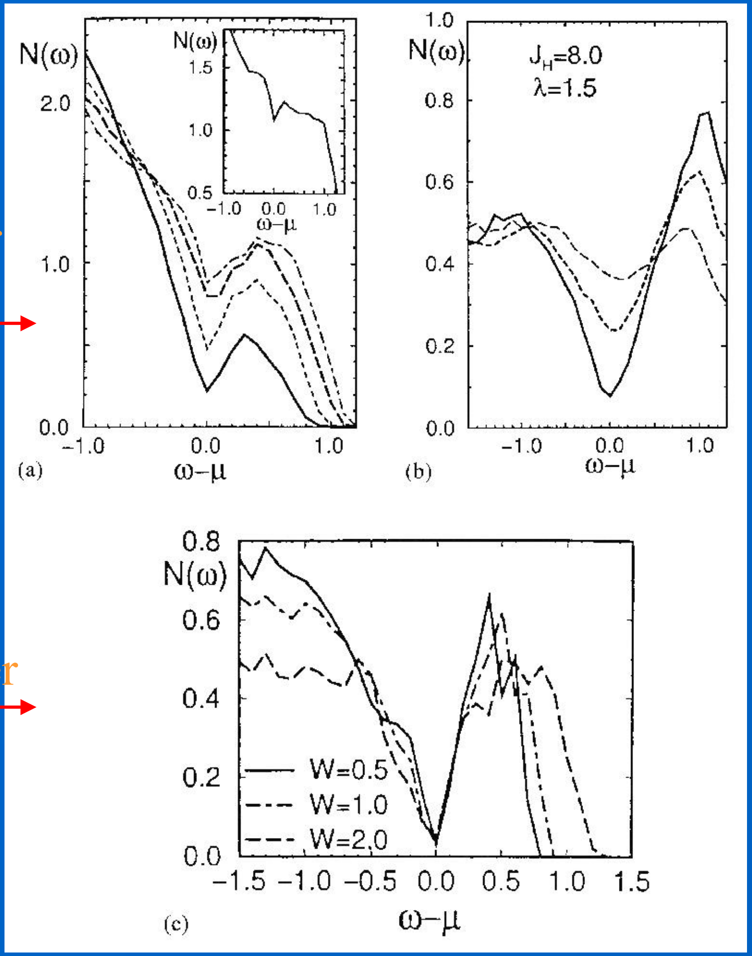
Clean-limit Tc.



# Pseudogap in simulations

No disorder

With disorder

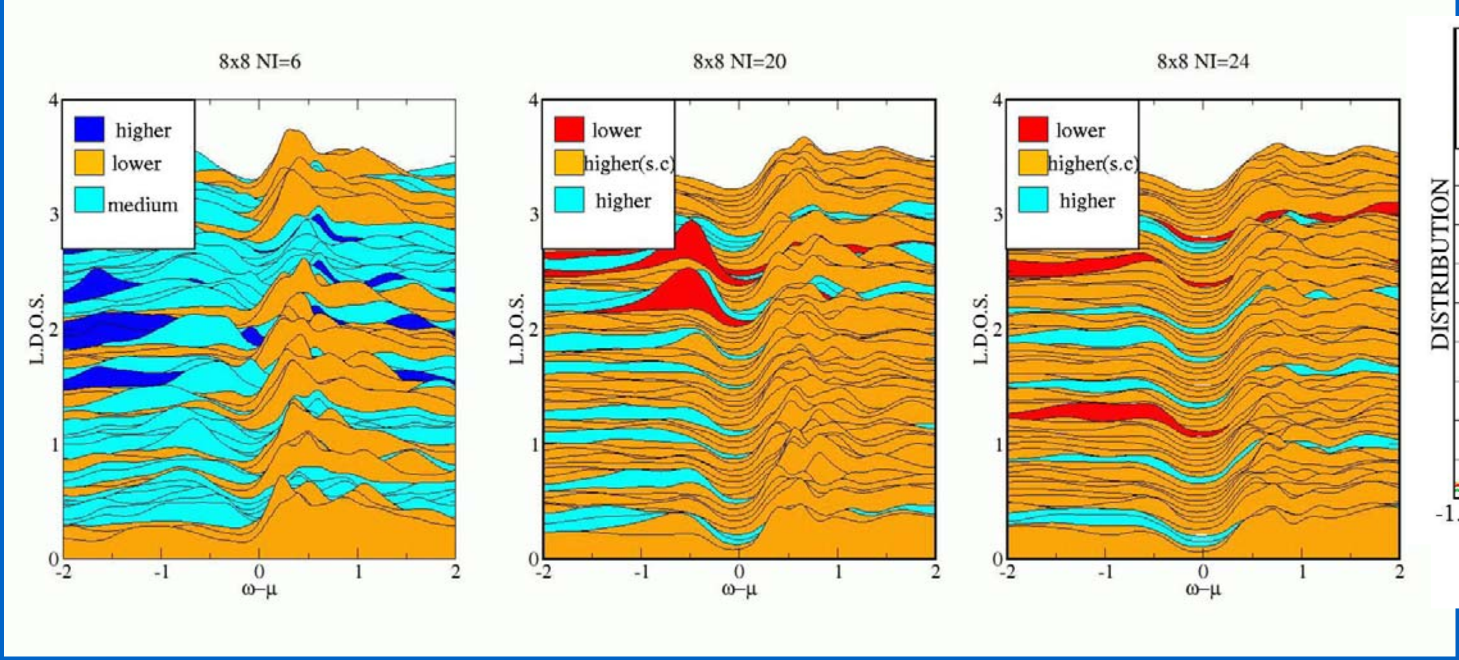


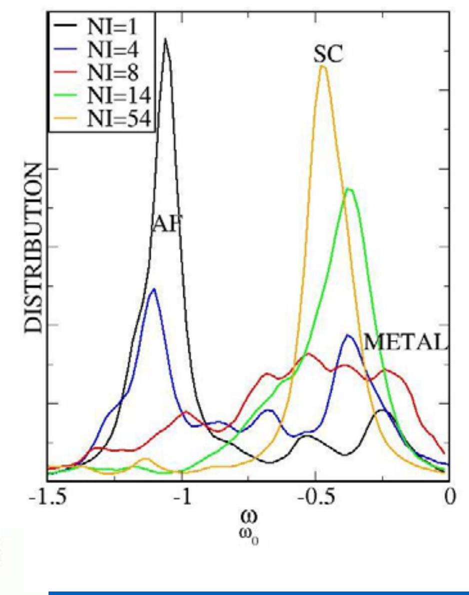

At intermediate temperatures dynamical clusters are found near the phase-separation critical temperature.
The clusters are metallic or insulating, inducing a Pseudogap. ← similarities with cuprates!

A.Moreo et al., PRL 83, 2773 (1999)

See also Dessau et al.
ARPES, bilayers
PG observed..

# Doping evolution of LDOS (in progress)




Glassy state (I)

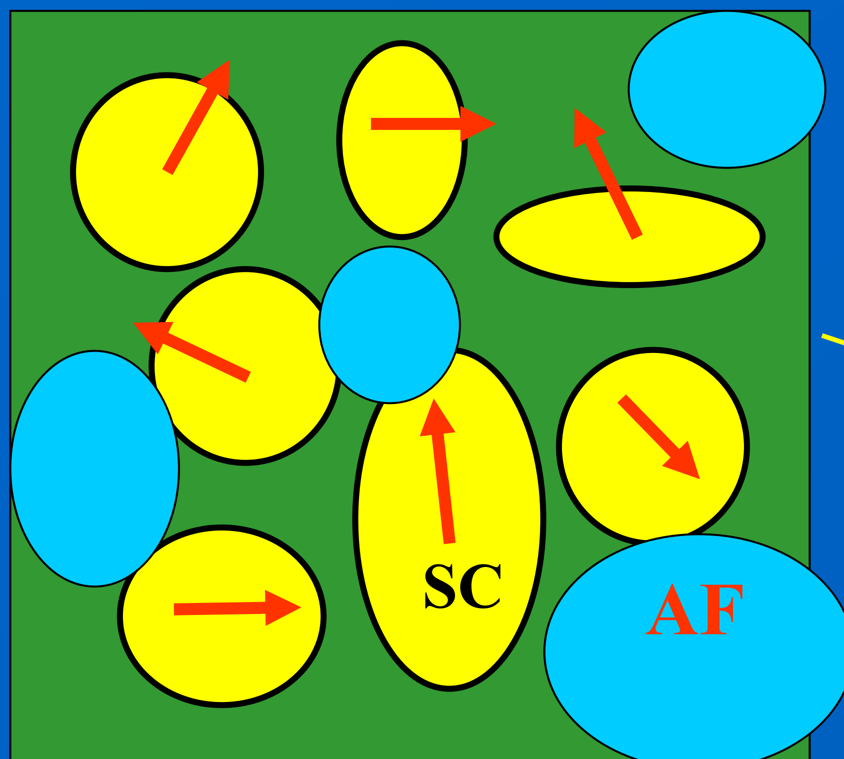
Lightly Underdoped (II)

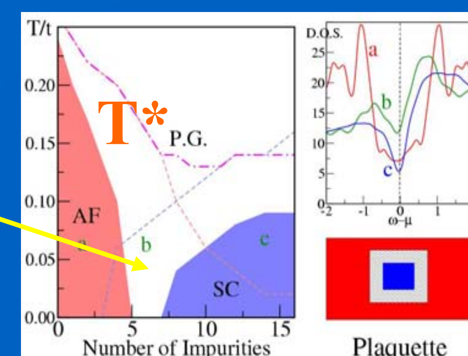
Optimal (III)

Distribution of LDOS gaps.

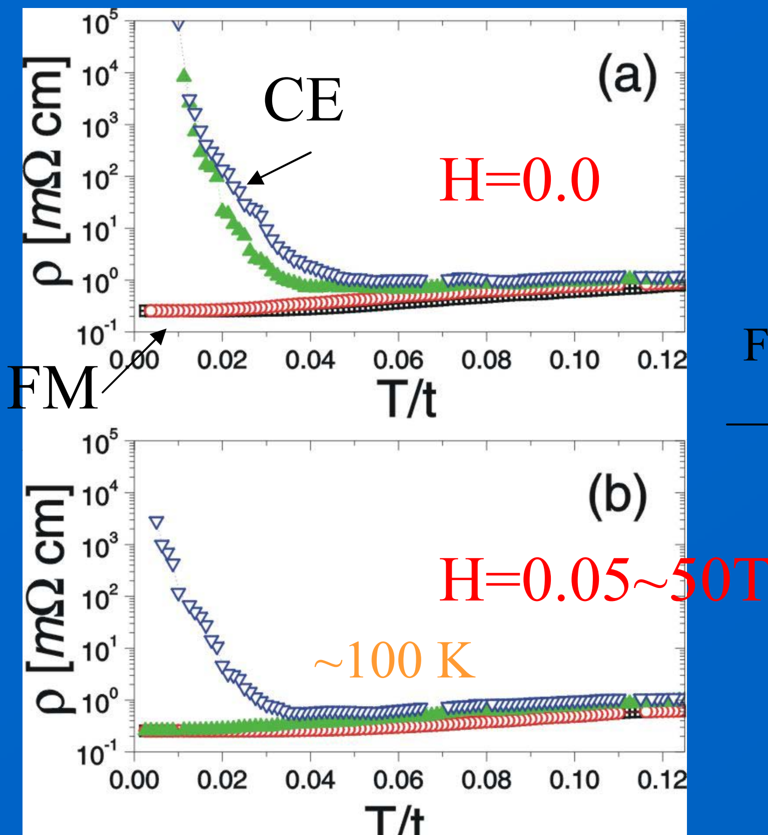
# Cartoonish version of MC results

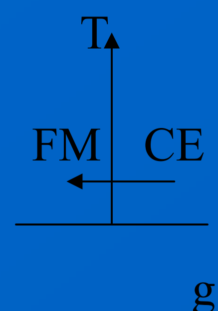
Random orientation of the local SC phases

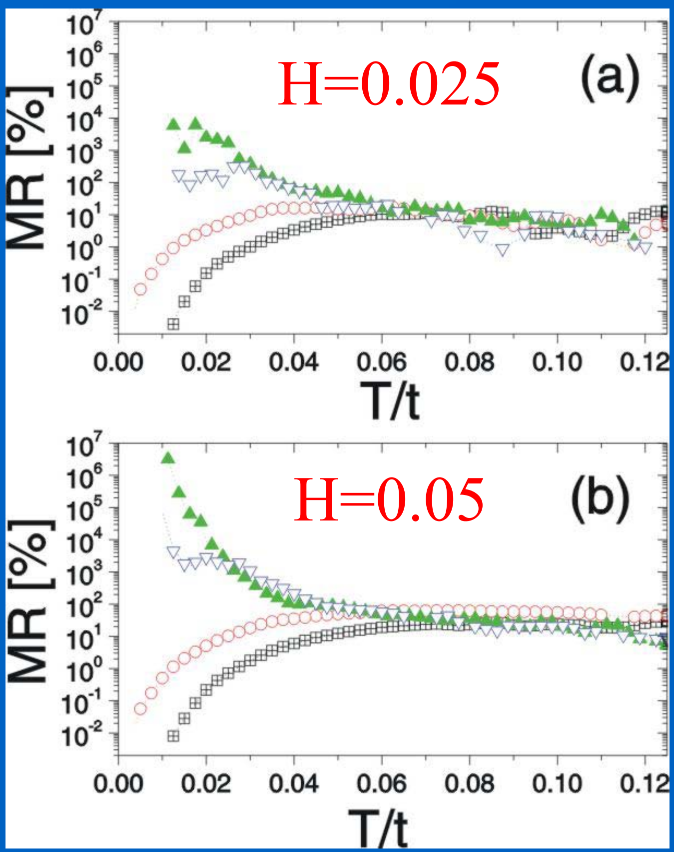


# New: CMR at low-T even in clean-limit, due to first-order transition FM-CO

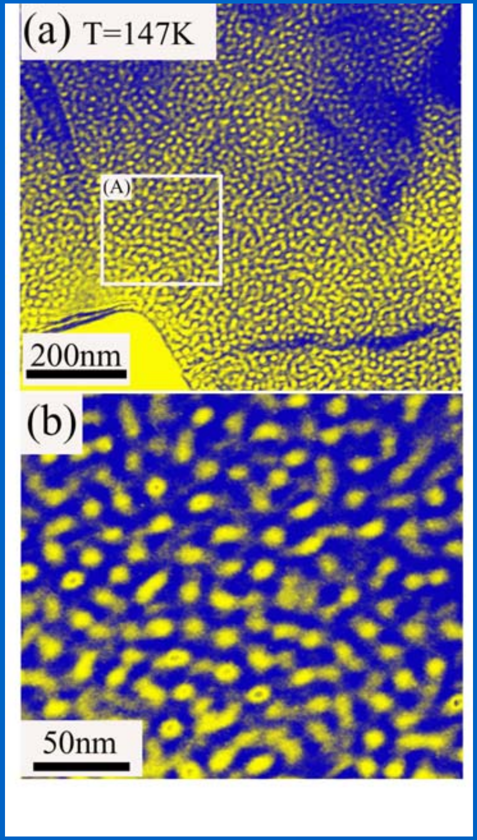



Aliaga et al., 4x4, x=0.5 Technique: lead-cluster-lead

# New Experimental Evidence




Mori, Cheong et al.
Lorentz microscopy

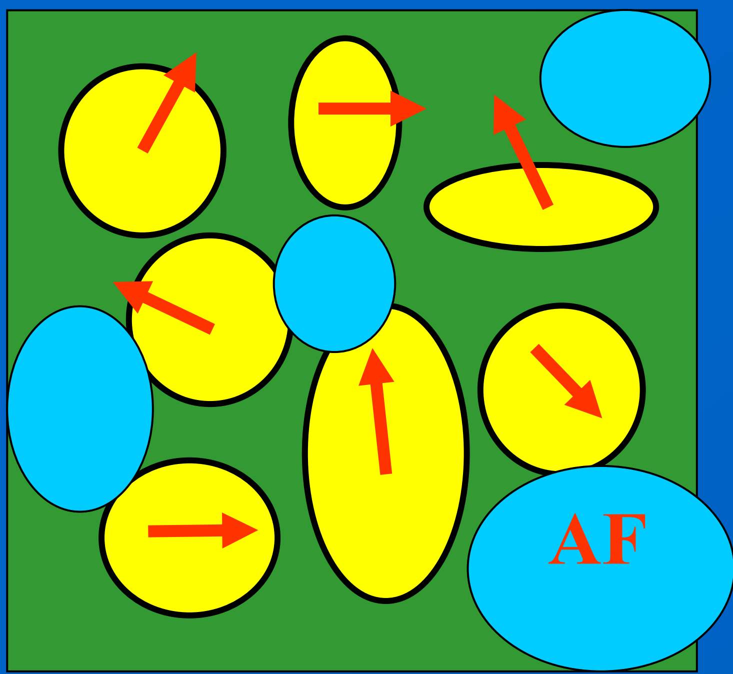
**FM nanodomains**

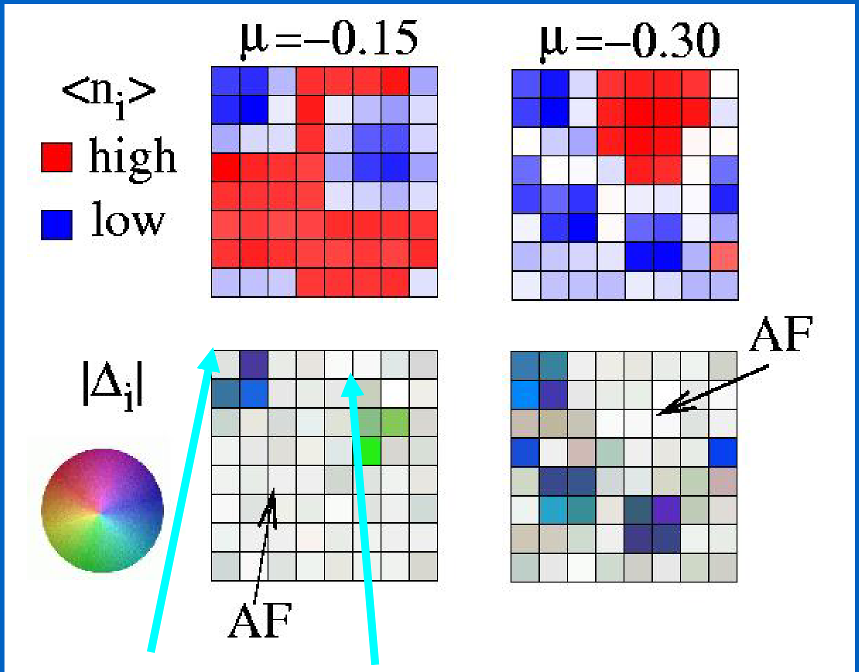
**Tc=85K, T*=170K**

$La_{0.25}\,\mathrm{Pr}_{0.375}\,Ca_{0.375}Mn\,O_3$

# Adding Coulombic centers
## (simulating Sr(2+)  in 214)

Phases of the local SC island

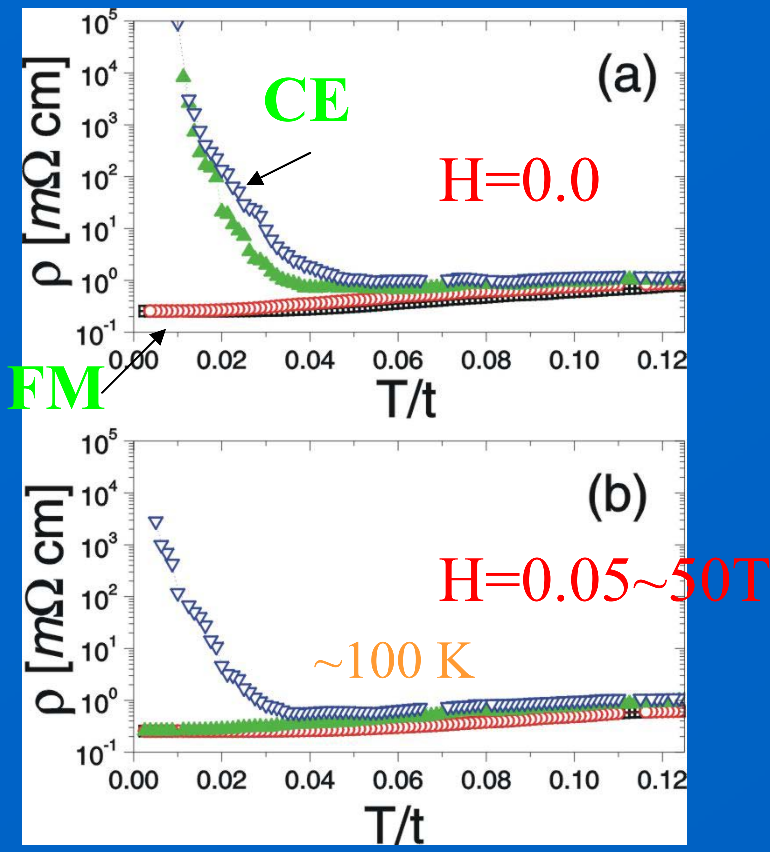


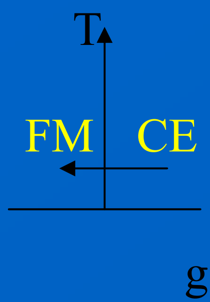

SC islands have different phases

# “Low-T CMR” appears in *clean-limit*, due to first-order transition FM-CE

(Aliaga et al., PRB 68, 104405 (2003))




x=0.5

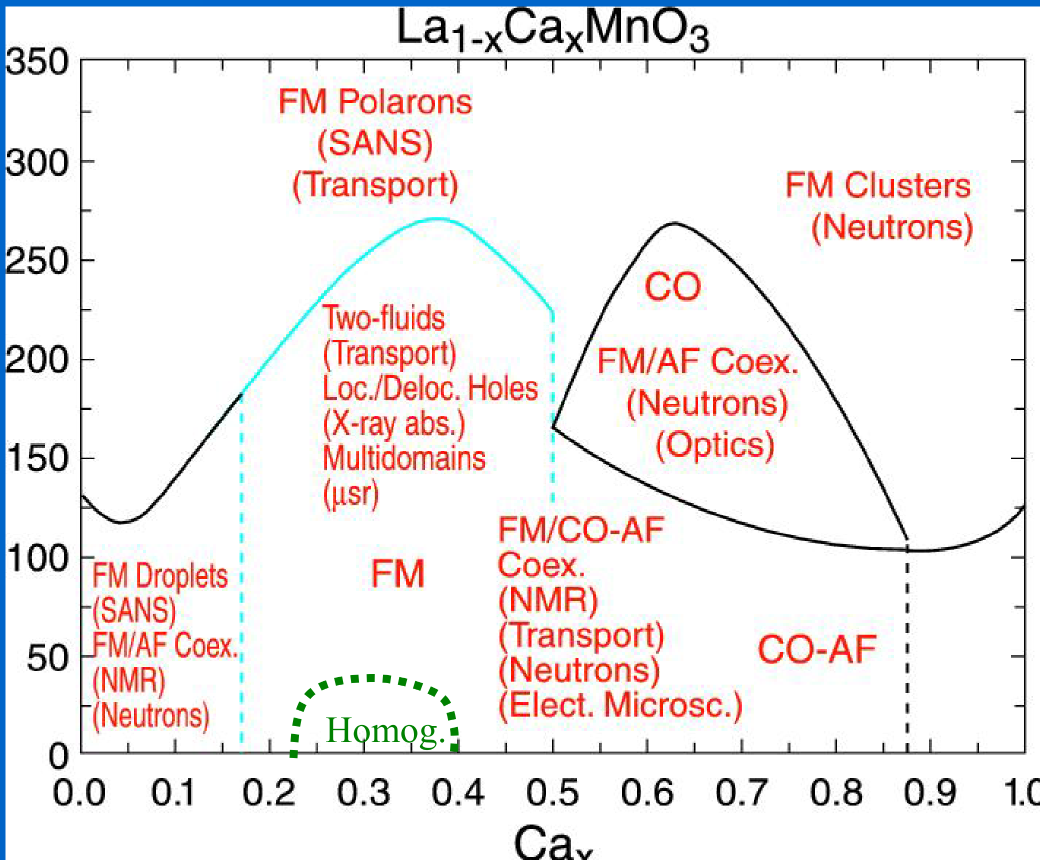




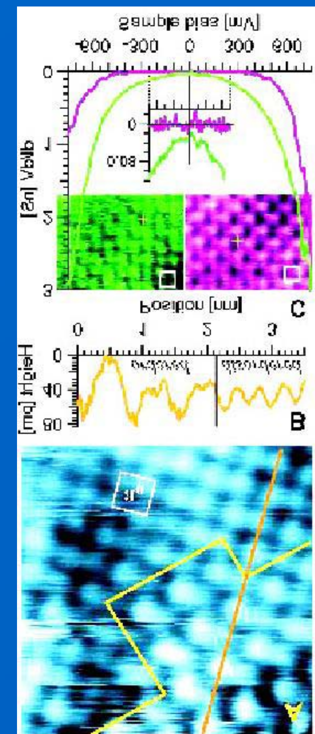
Technique: lead-cluster-lead

Standard CMR?

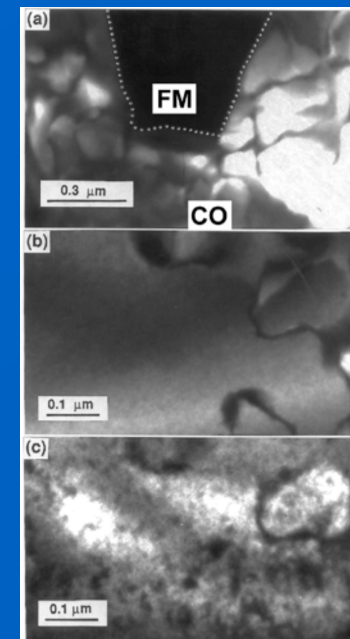
# Recent Trends: Phase Coexistence in Manganites




A.Moreo et al.,
Science 283, 2034 (1999).



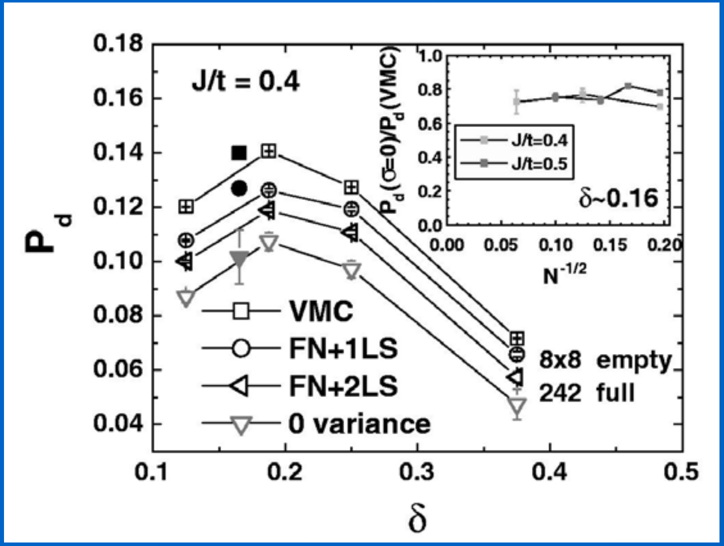
Renner et al.,
Nature '02
BiCaMnO
STM




Uehara et al.,
Nature '99
LaPrCaMnO
EM

# (II) High-temperature superconductivity

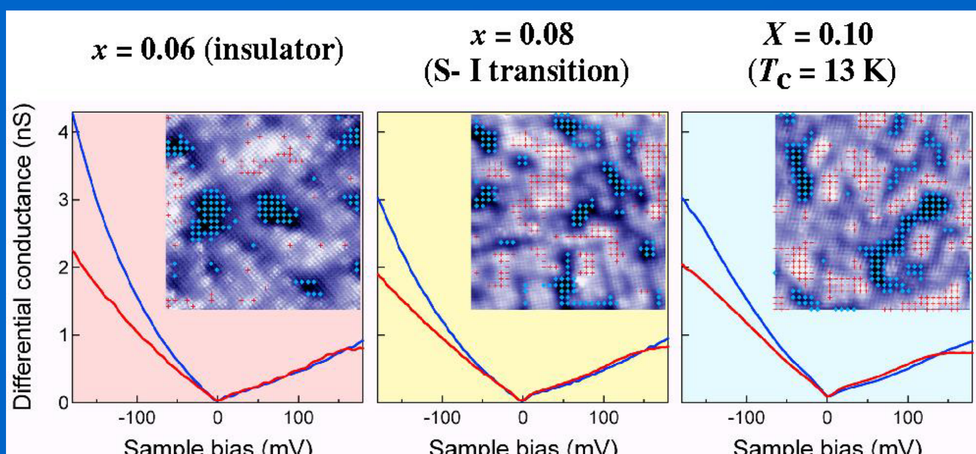
Sorella et al., PRL 88, 117002 (2002)

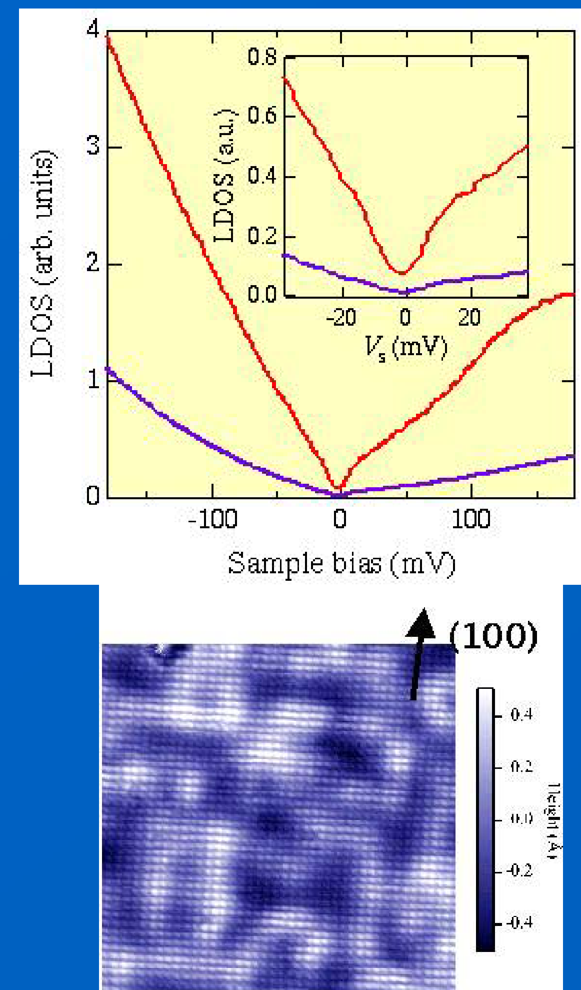



**SC appears in t-J simulations due to short-range AF, as in 2-leg ladders**
**However, other studies show stripes.**
**SEVERAL PHASES IN COMPETITION.**

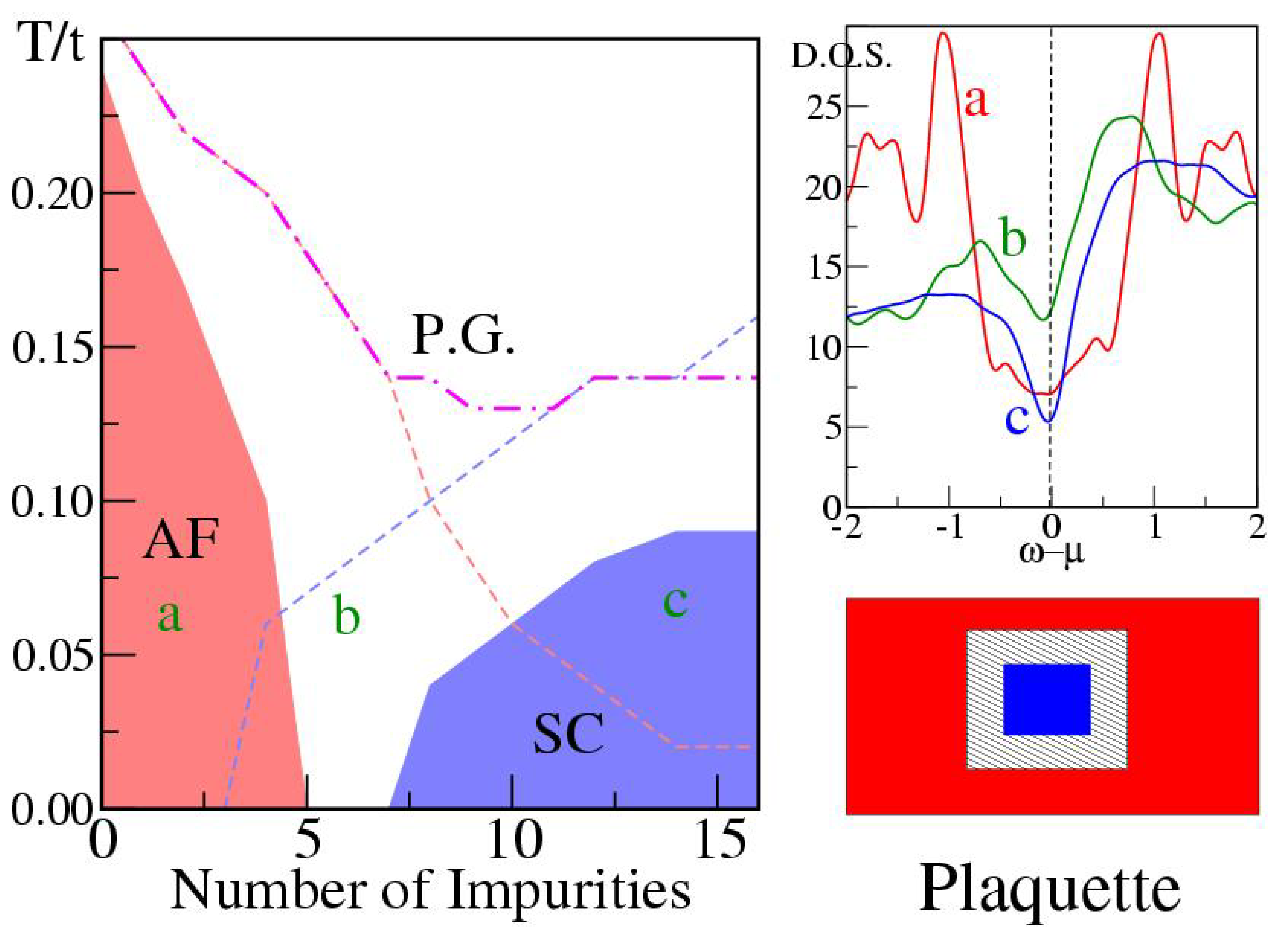
# STM for $Ca_{2-x} Na_x Cu O_2 Cl_2$

## (Takagi's group, unpublished)

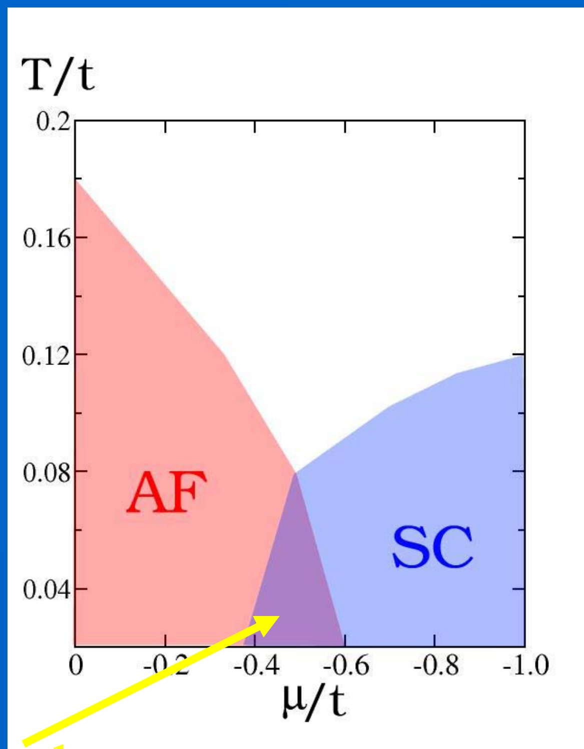


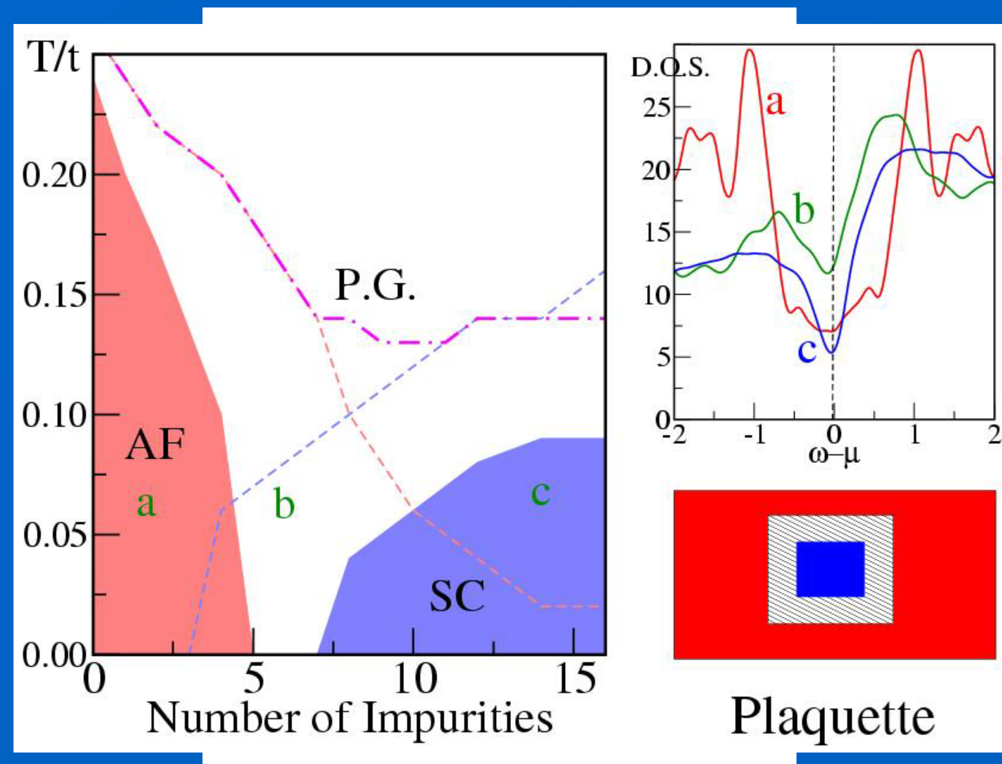

**Inhomogeneities both before and after the SC-Insulator transition. A percolation appears to occur?**


T/t
0.20
0.15
0.10
0.05
0.00
0
5
10
15
Number of Impurities
P.G.
AF
a
b
c
SC
D.O.S.
25
20
15
10
5
0
-2
-1
0
1
2
ω−μ
a
b
c
Plaquette

# Quenched disorder leads to clusters and T*, as in manganites.




tetracritical




Without disorder

With Coulombic disorder

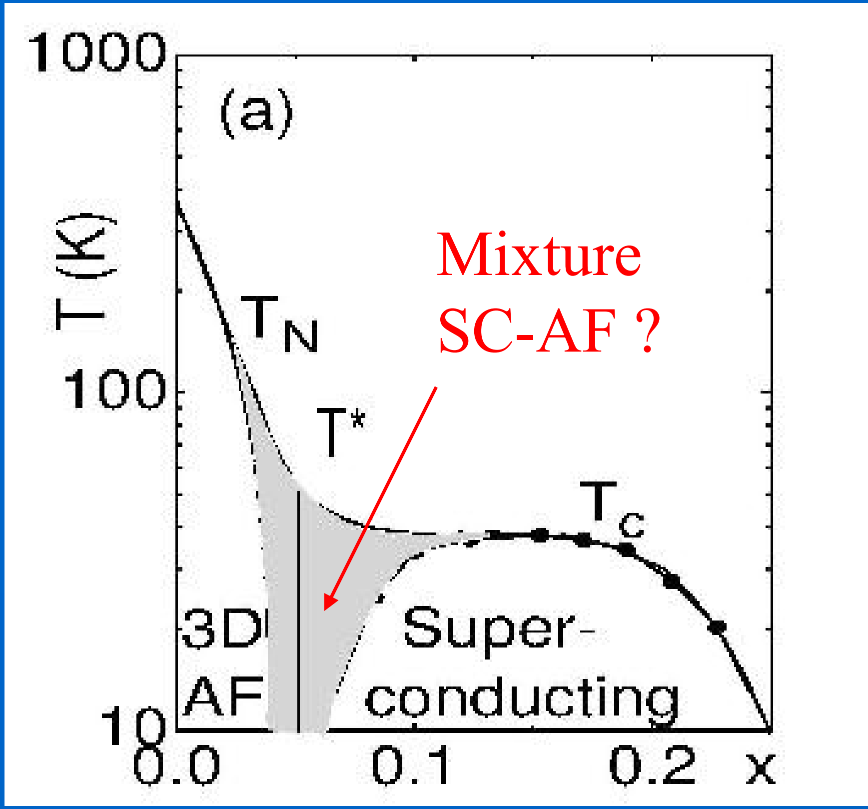
# Inhomogeneities =>
# Complexity in transition-metal oxides?

- ``Complex systems exist on the edge of chaos – they may exhibit almost regular behavior, but also can change dramatically and stochastically in time and/or space as a result of small changes in conditions.''

T. Vicsek, Nature 418, 131 (2002).

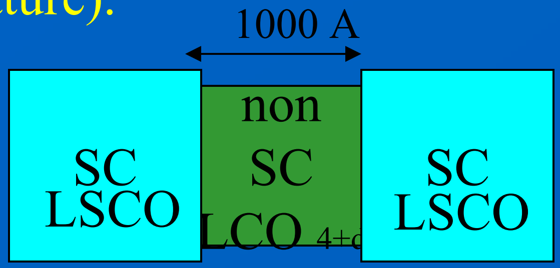
**First-principles approaches may not work.**
**Computational work is important in this context.**
**Large scale phenomenological models will be needed.**

# CMR-motivated Speculations for Cuprates:



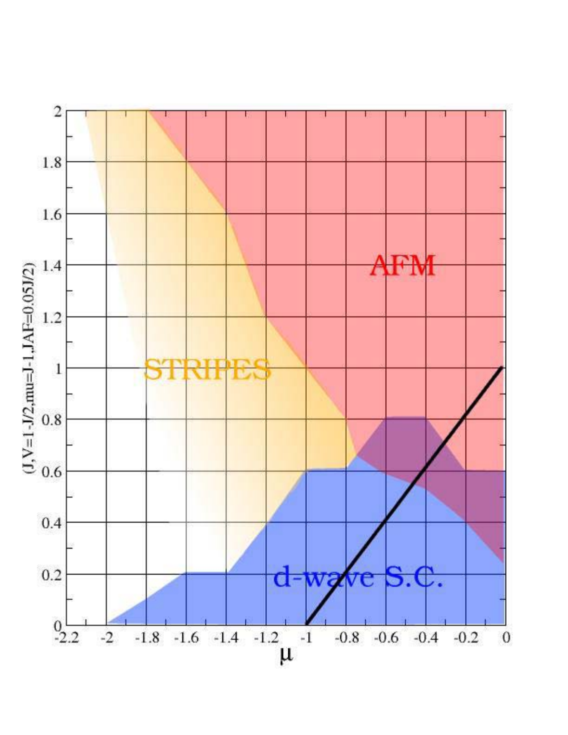

PRL 87, 277202 (2001)

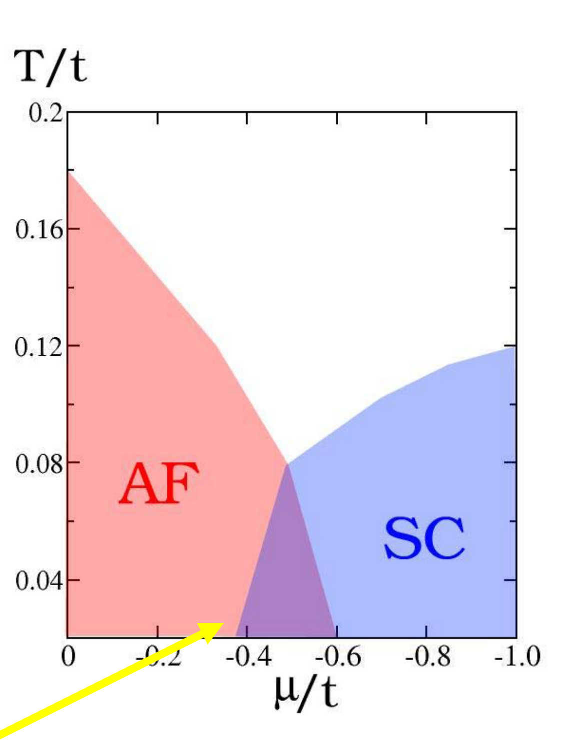
- First-order AF-SC transition in clean limit?
- Percolative transition? T* as a Griffiths T? "Colossal" Effects in underdoped regime? (``Giant proximity effect'' reported by Decca et al.PRL, and Bozovic et al. submitted to Nature).

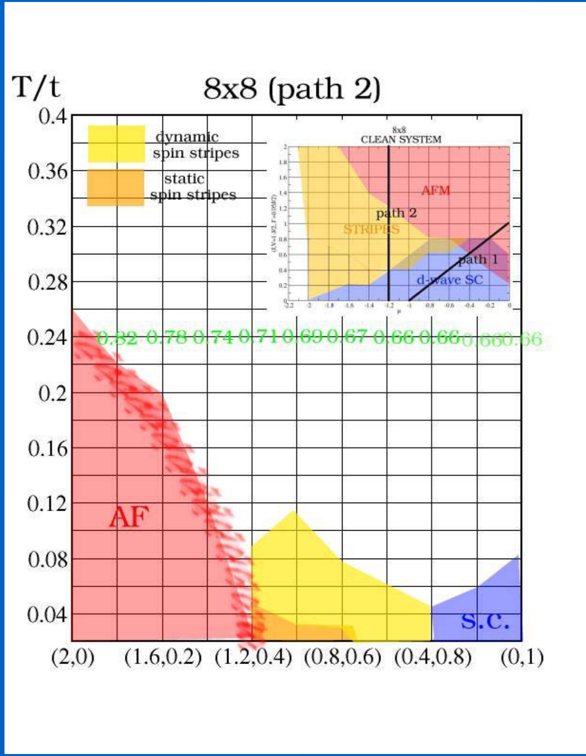


# In progress: SC vs. AF competition

**MC results for mean-field model of electrons coupled to classical AF** (Moreo et al., PRL 88, 187001 (2002)) **and SC order parameters** (Alvarez et al., in preparation)



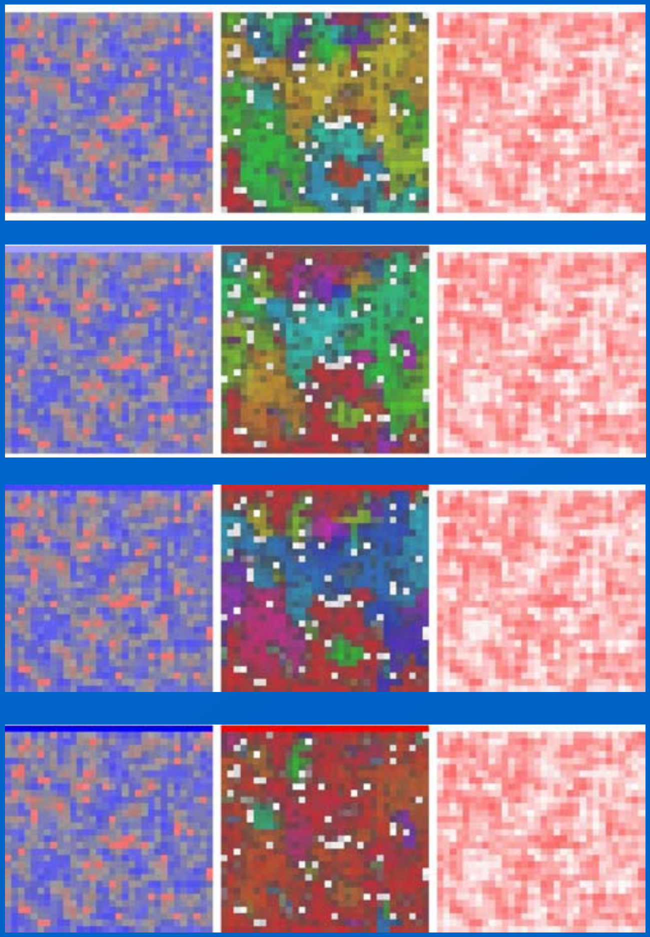




tetracritical

Without disorder

Without disorder

# Giant Proximity Effects?
## (through boundary, as in Josephson junctions)



D_top=0

D_top=1

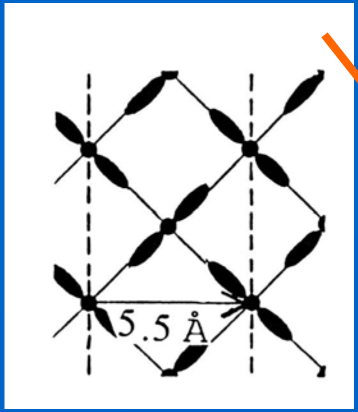
D_top=2

D_top=2.8

u_12=0.7, beta=100, 32x32,W=0.7
rho2=0.3

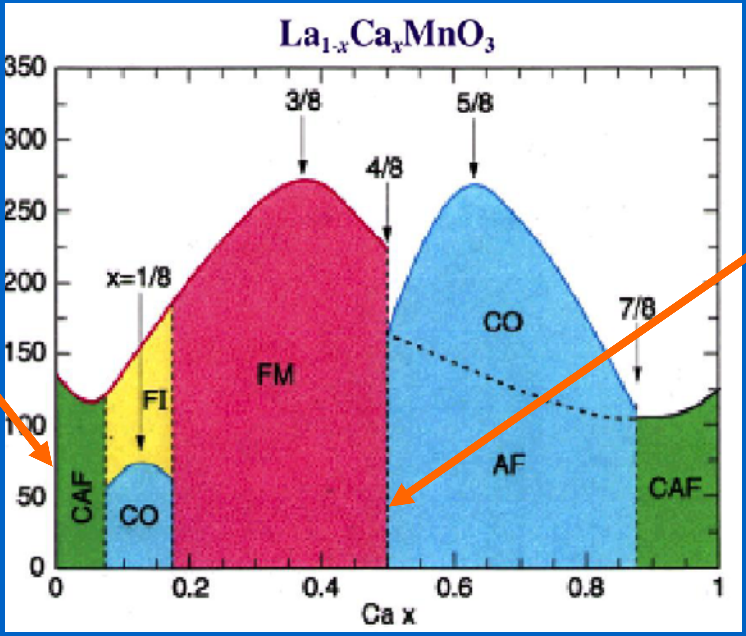
# Motivation II:

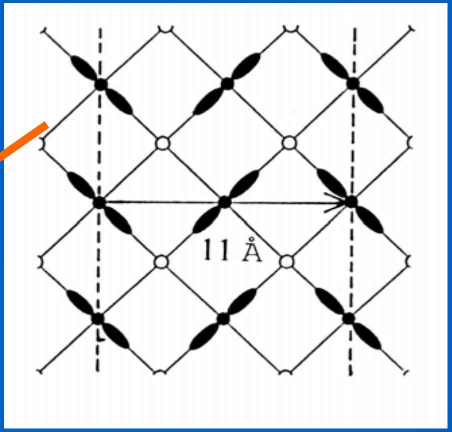
- Understand the rich phase diagram that experiments are unveiling.




A-type AF
Orbital order

T



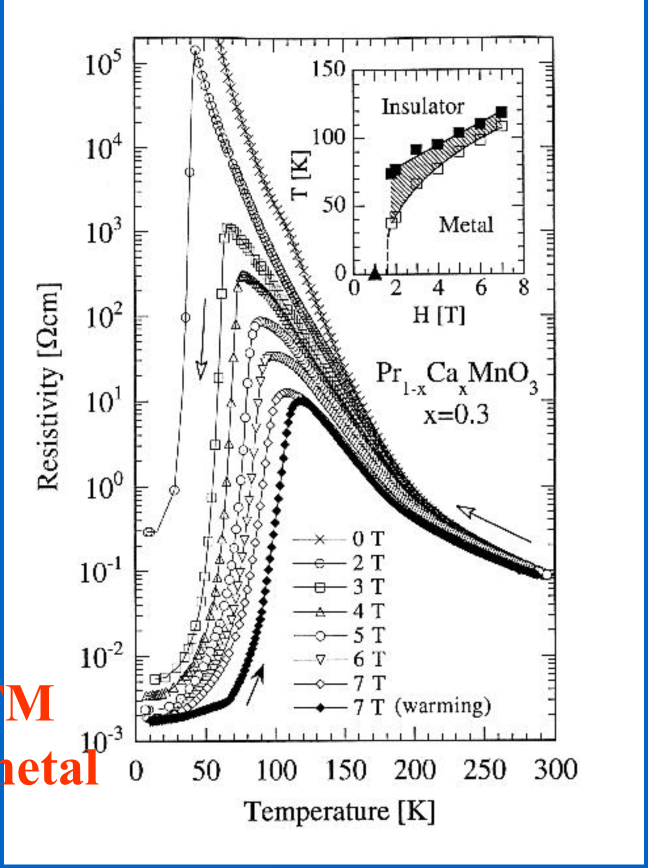




CE-type
Spin/charge/orbital order

Cheong et al.,
Schiffer et al.

Fraction of holes

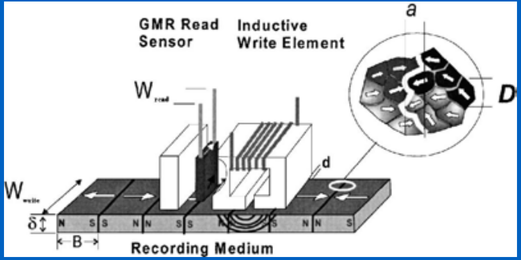
# Motivation I: Colossal Magnetoresistance (CMR)



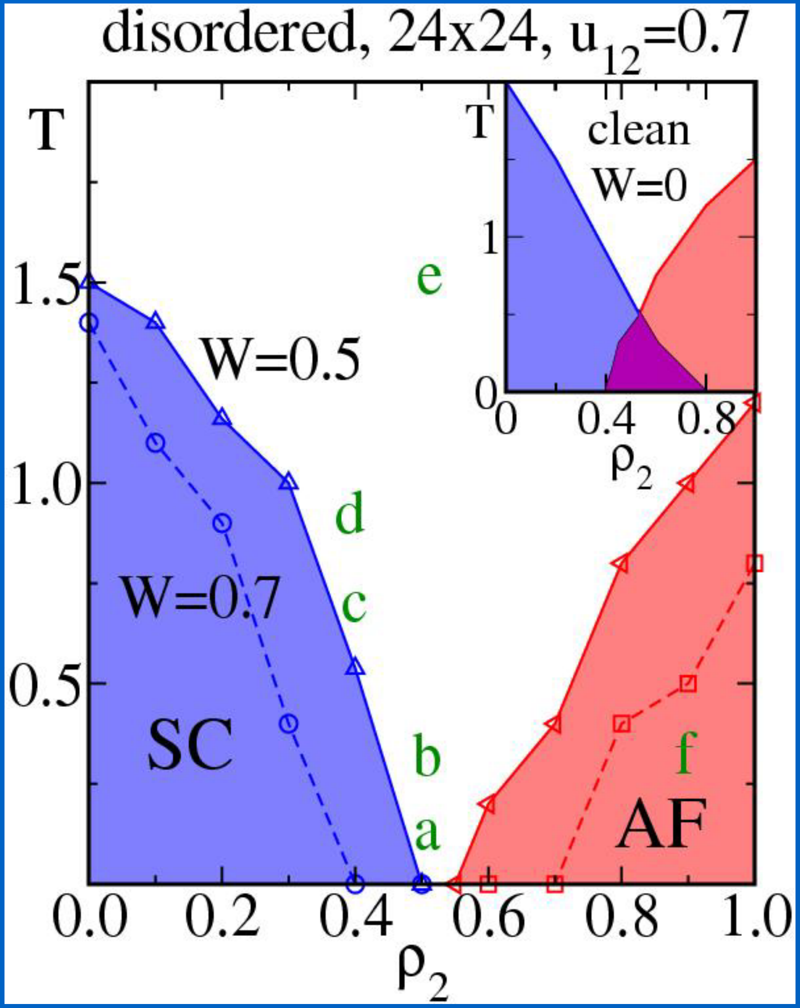

FM metal

- Drastic reduction of resistivity with small magnetic fields. Potential application in "read sensors"?

Tomioka and Tokura, (1999).

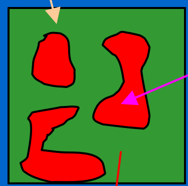


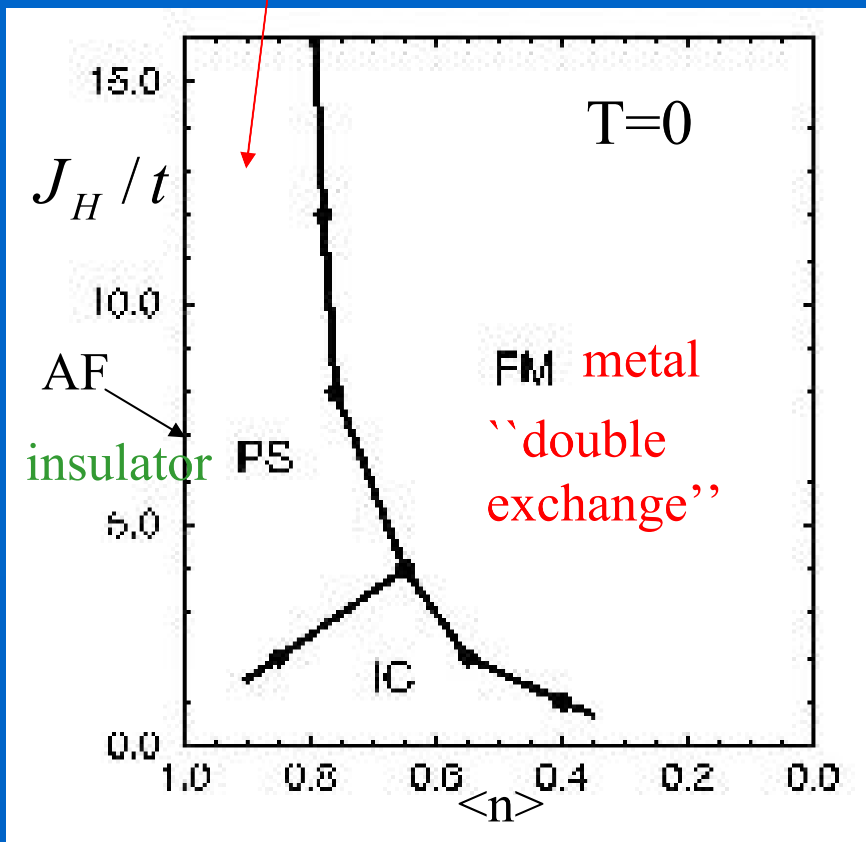

1 bit ~ 100nm x 100nm


disordered, 24x24, $u_{12}$=0.7
T
1.5
1.0
0.5
0.0
0.2
0.4
0.6
0.8
1.0
$\rho_2$
W=0.5
W=0.7
SC
AF
a
b
c
d
e
f
clean
W=0
1
0
0.4
0.8

# Typical MC results

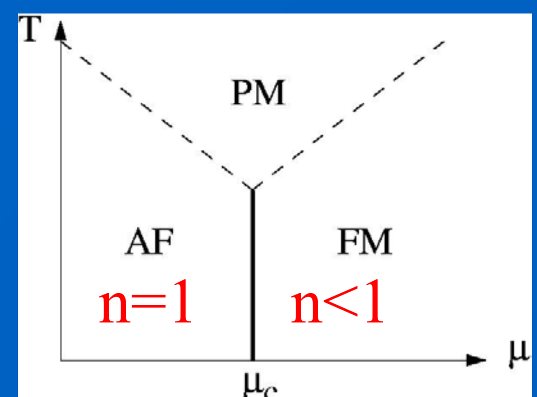
AF As observed experimentally (see later)



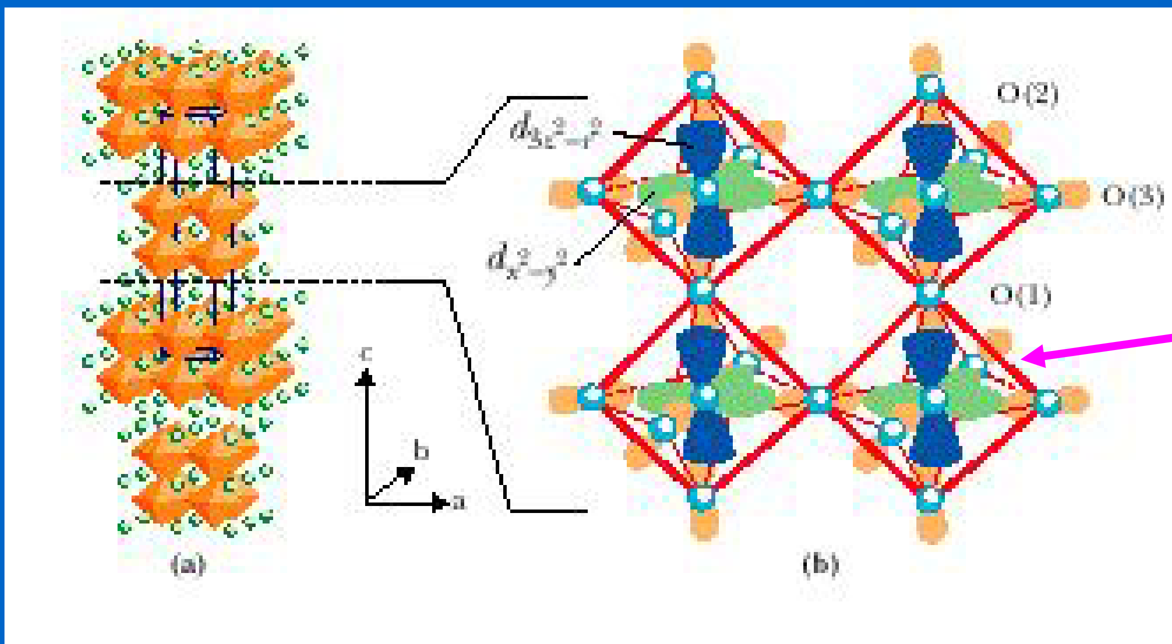

Yunoki et al. PRL80, 845 (1998).

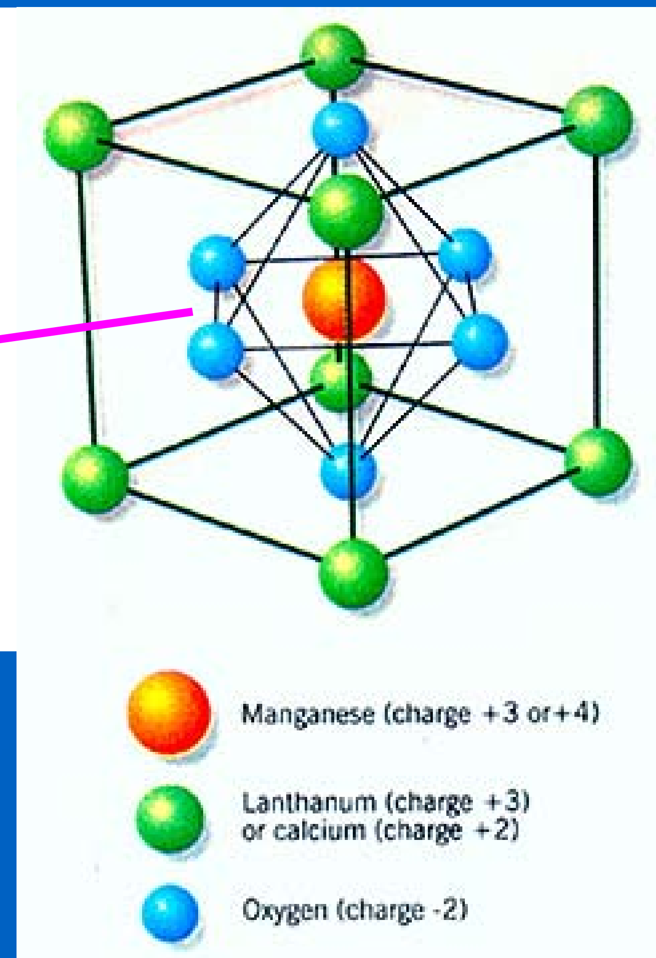
- FM, AF , Phase Separation and Spin Incommensuration observed.




AF-FM are first-order transitions in many other cases

# Structure of the Manganites

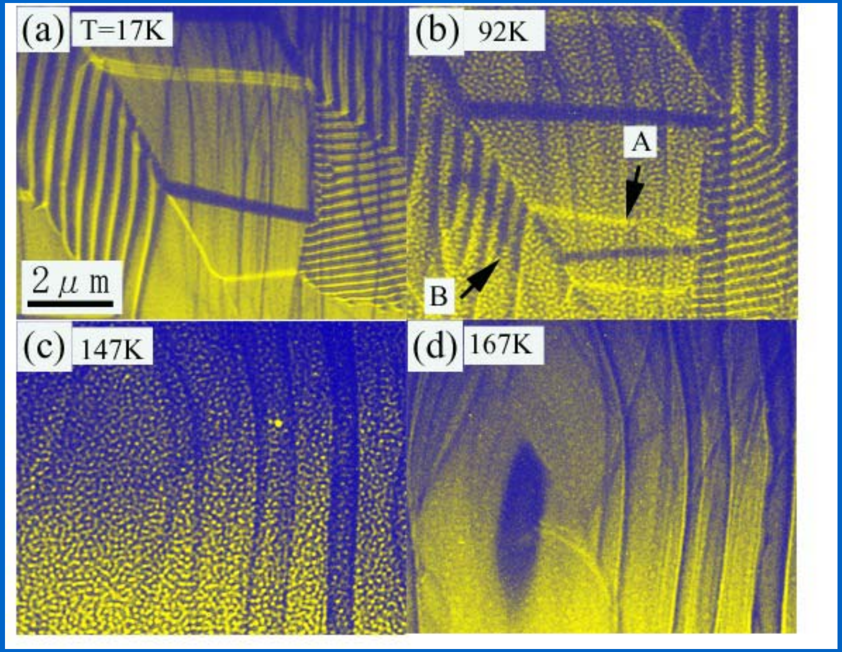



Bilayer $(La,Sr)_3Mn_2O_7$ n=2

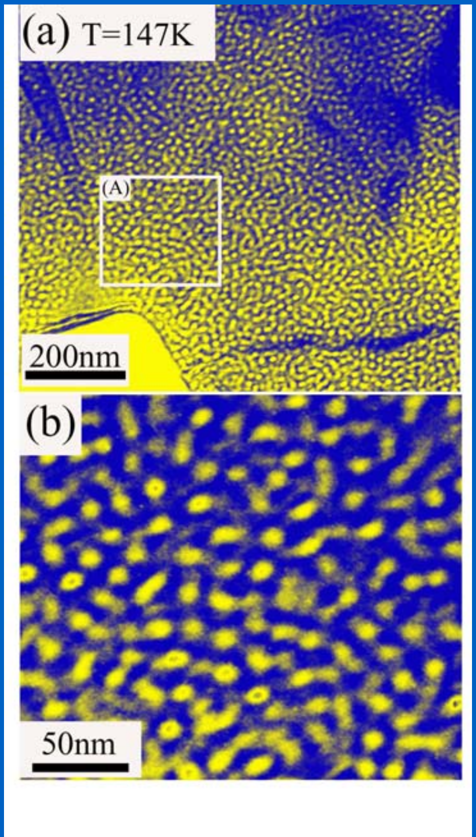
$$(R,D)_{n+1}Mn_nO_{3n+1}$$

# New Experimental Evidence




Mori, Cheong et al.
Lorentz microscopy

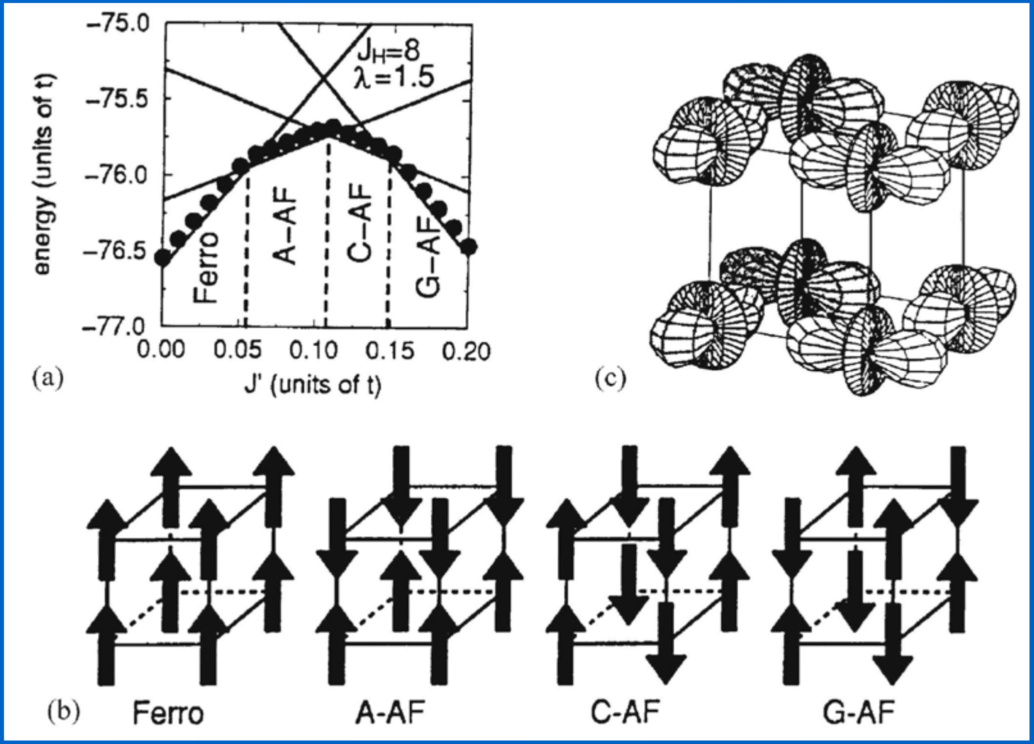
$La_{0.25}\,Pr_{0.375}\,Ca_{0.375}MnO_3$




**See also Ma, Gai, Torija, Plummer, and Shen, STM, preprint.**

**FM nanodomains**
**Tc=85K, T*=170K**

# Orbital and Spin order at x=0




Hotta et al.
PRB 60, R15009
(1999)

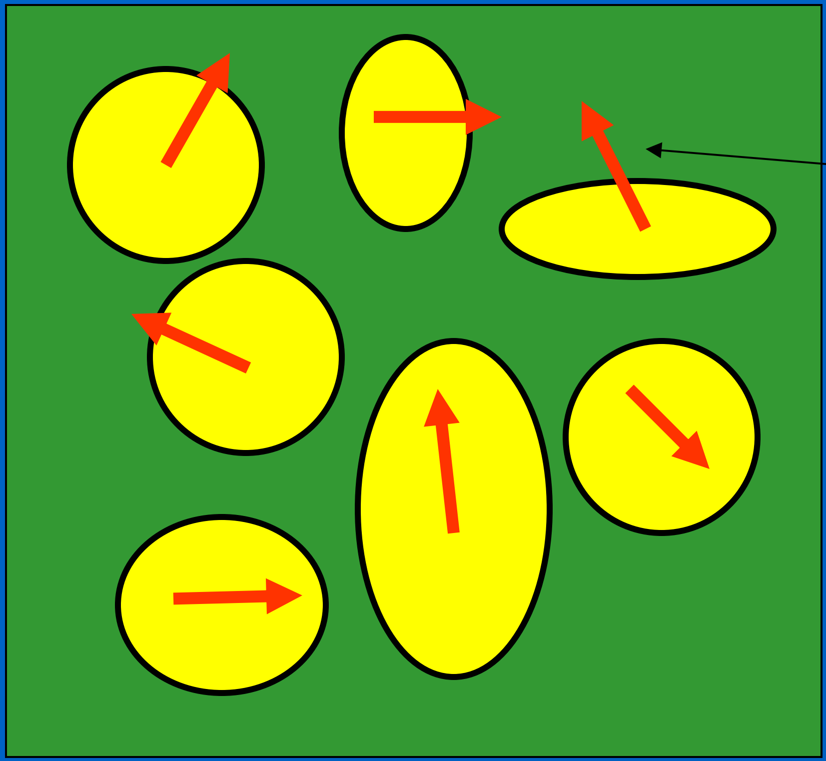
Spin and orbital order at x=0

Many states close in energy => JAF is much relevant.

# Conclusions

- Experiments + theory have revealed nano-scale inhomogeneities in TMOs. Disorder and intrinsic PS tendencies are at work.
- Phase competition emerges as a key concept in correlated electron systems. Complexity appears to occur in TMO, and causes CMR and possibly other colossal effects.
- Disorder cannot be neglected in many compounds.

# Cartoonish view of ``preformed'' SC islands state (``phase glass'')



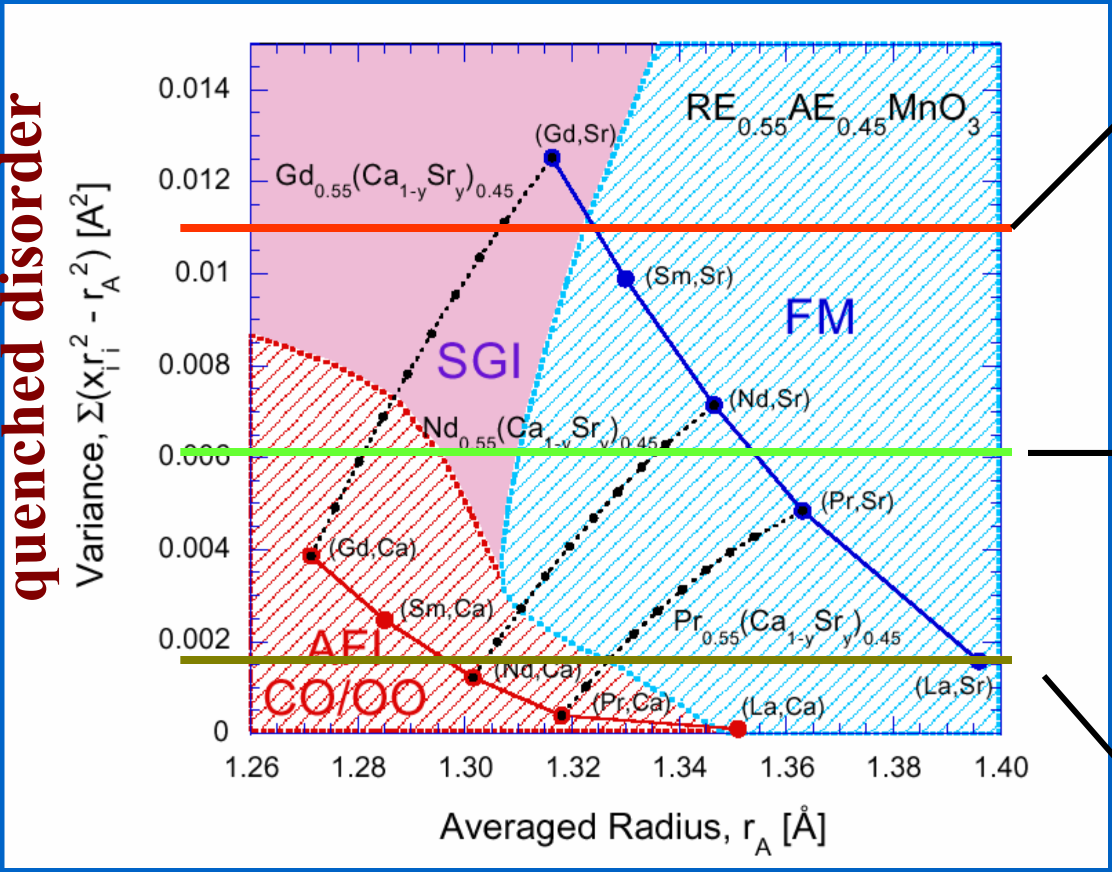
**Phase of the local SC island**

Very different from preformed-pairs view.

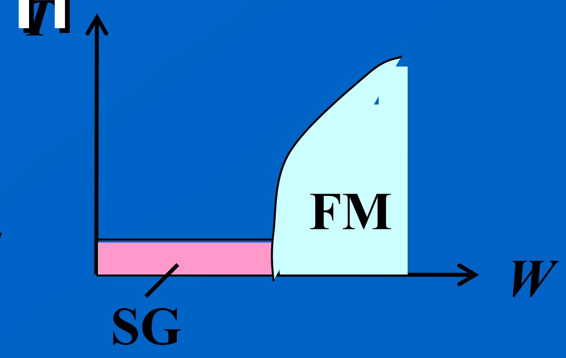
Experiments?

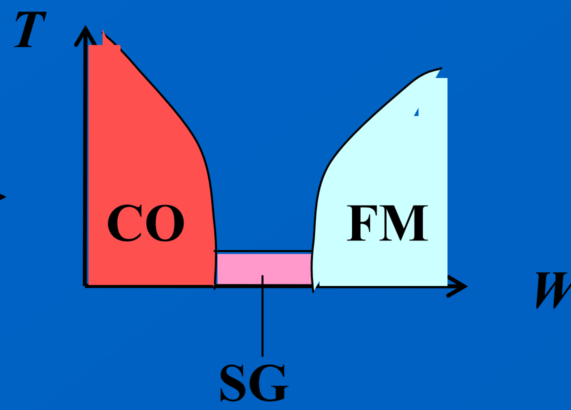
# Global Phase Diagram

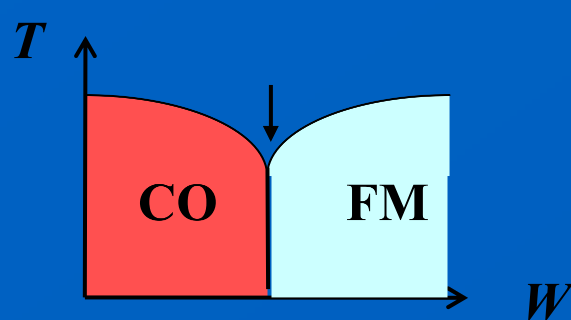
quenched disorder




bandwidth *W*



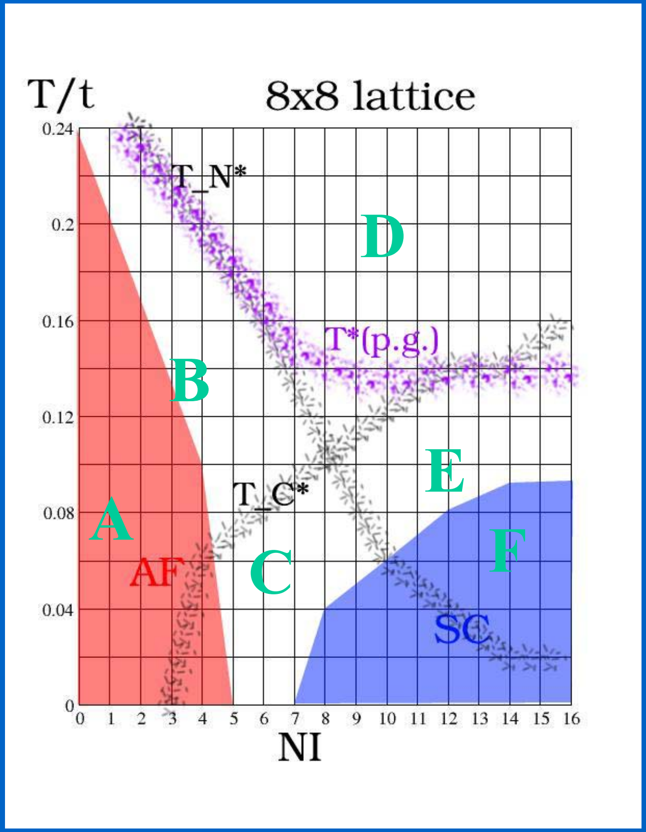



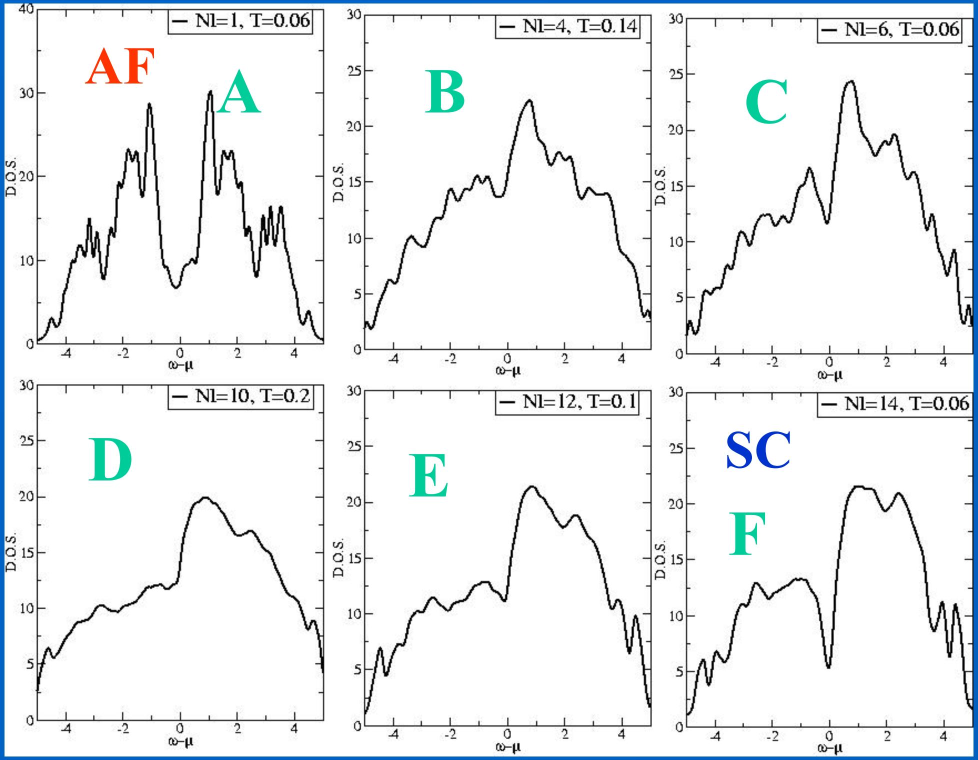




quenched disorder

Tokura et al.. See PRL 2003.

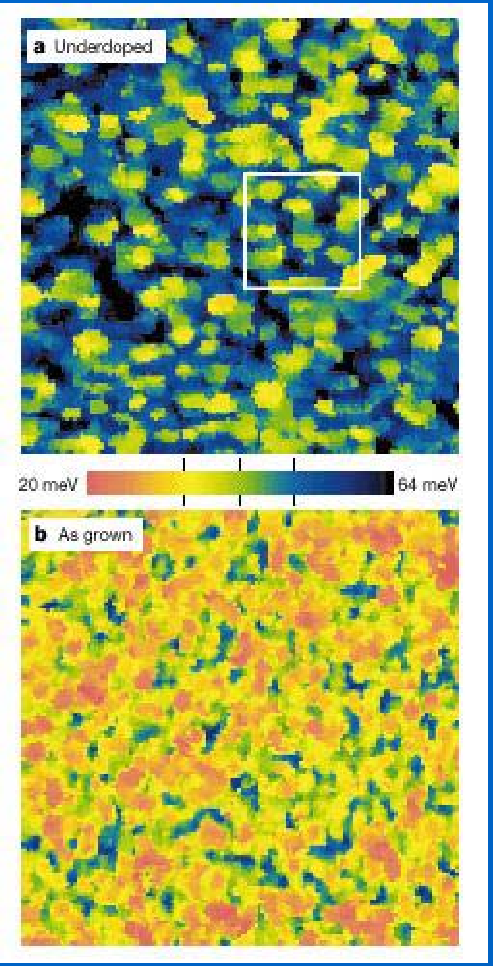
# Density of states and pseudogaps



# Recent trends in High-Tc Cuprates: STM Gap Maps

560A
x
560A




Underdoped Bi-2212, Tc=79K

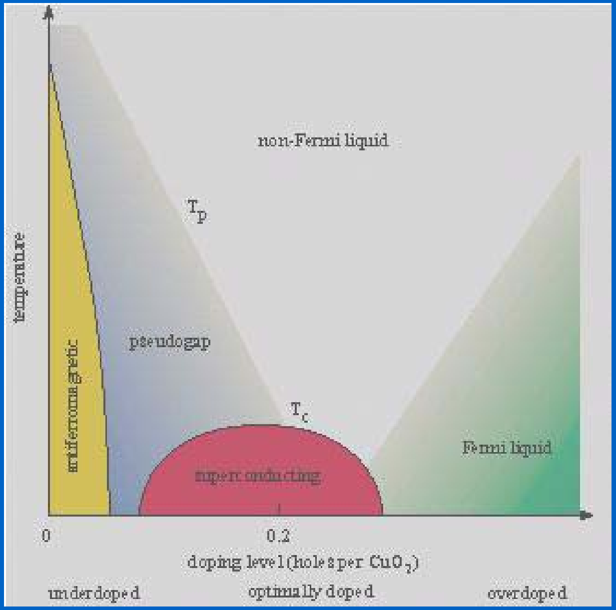
Overdoped Bi-2212

- Mixture of two different short-range electronic orders?
- Long-range characteristics of granular SC?
- SC domains ~3nm.

Lang et al., Nature ’02.
Davis, Pan, Uchida, …

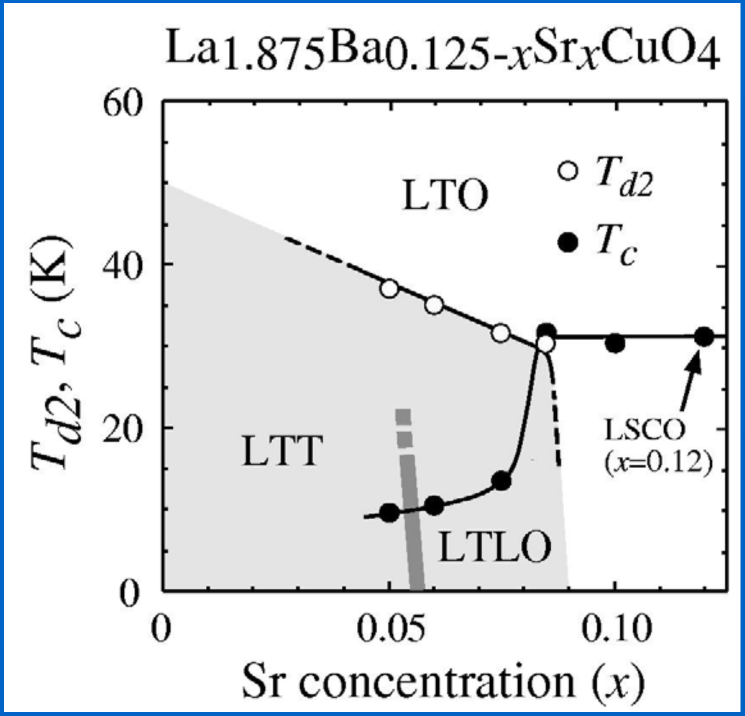
# High Temperature Superconductors

- Discovered in 1986
- Still not understood!
- Many proposals assume homogeneous states

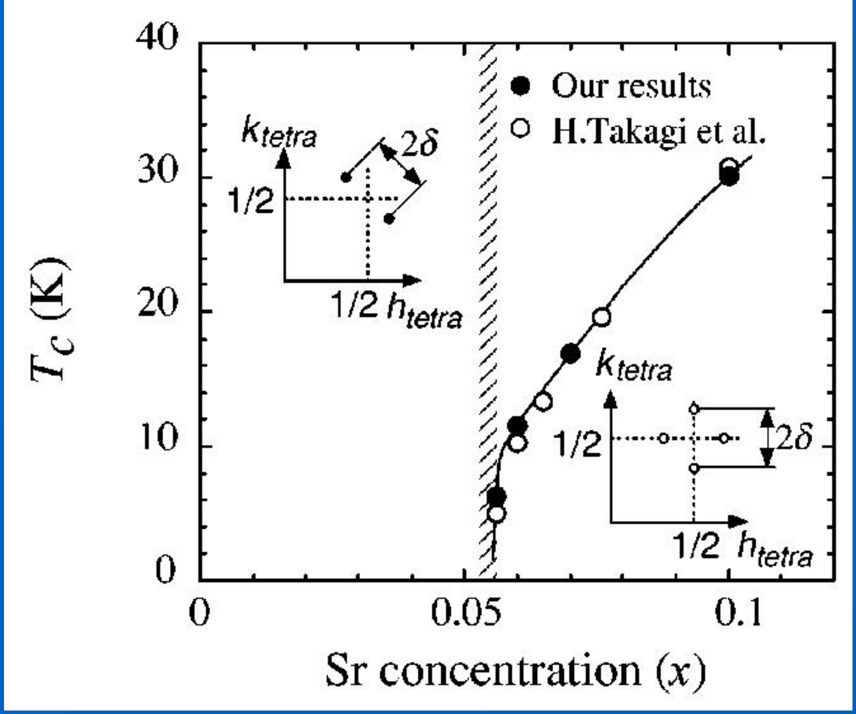



- **D-wave SC.**
- **Pseudogap**
- **Stripes?**

# First-order transitions in cuprates?

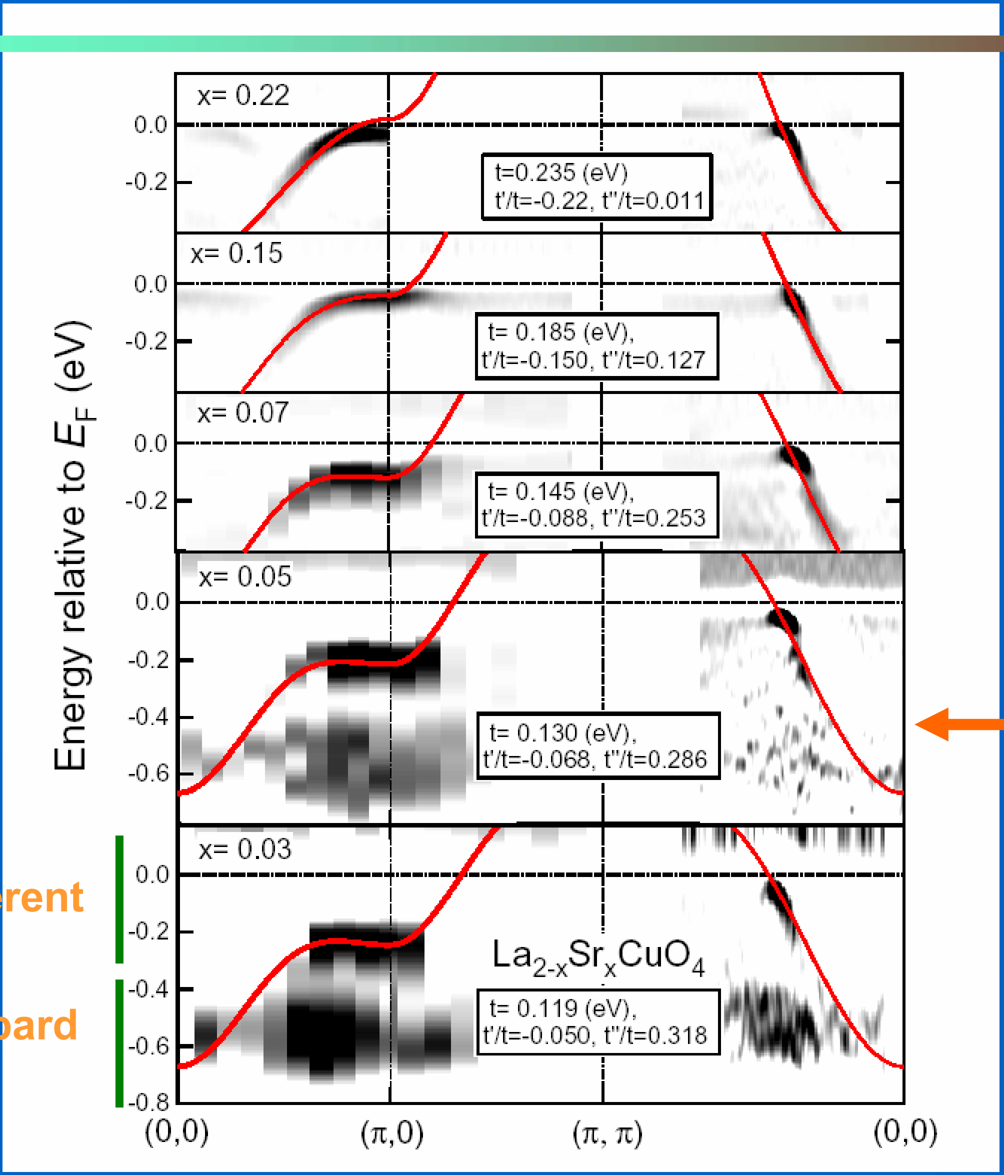



Fujita et al., PRL88, 167008 (2002)




LSCO, Fujita et al., PRB65, 064505 (2002)

# "Band structure" of $La_{2-x}Sr_xCuO_4$




coherent

Lower Hubbard

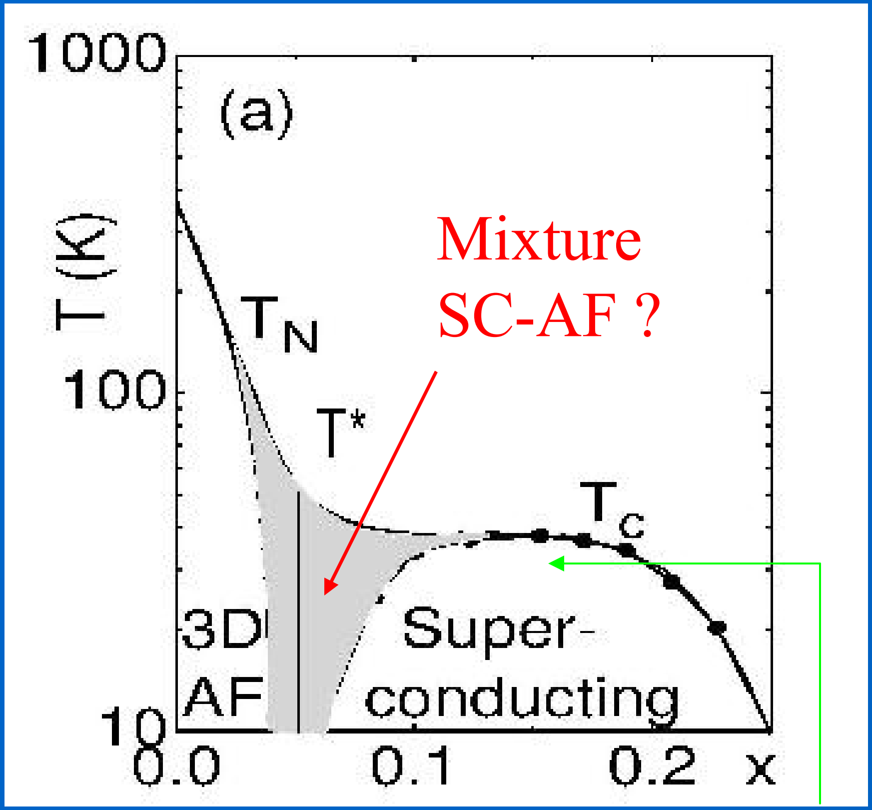
**See also Fujita et al., Yamada et al., …**
**Electron-doped, Organic SC, …**

Coexistence of two signals

tight-binding fit

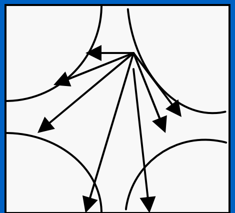
T. Yoshida et al., PRB '01 and unpublished

# CMR-motivated Speculations for Cuprates:




- First-order AF-SC transition in clean limit? Similar ideas in SO(5) context.
- Percolative transition? T* as a Griffiths T?
- "Colossal" Effects in underdoped regime? (``Giant proximity effect'' reported by Decca et al.PRL, and Bozovic et al. submitted to Nature).

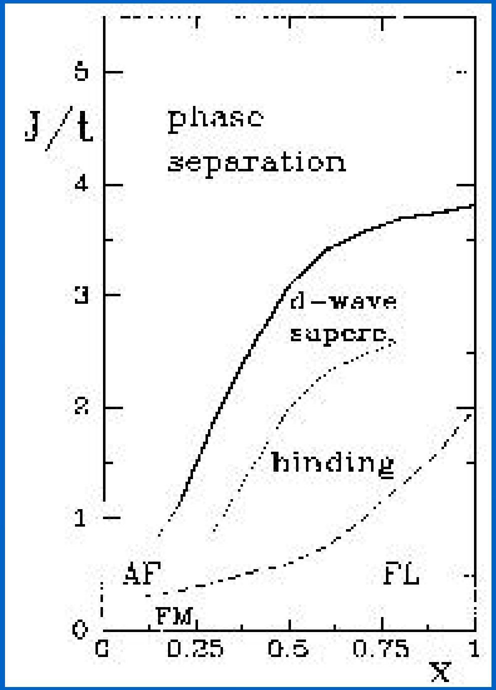
PRL 87, 277202 (2001)



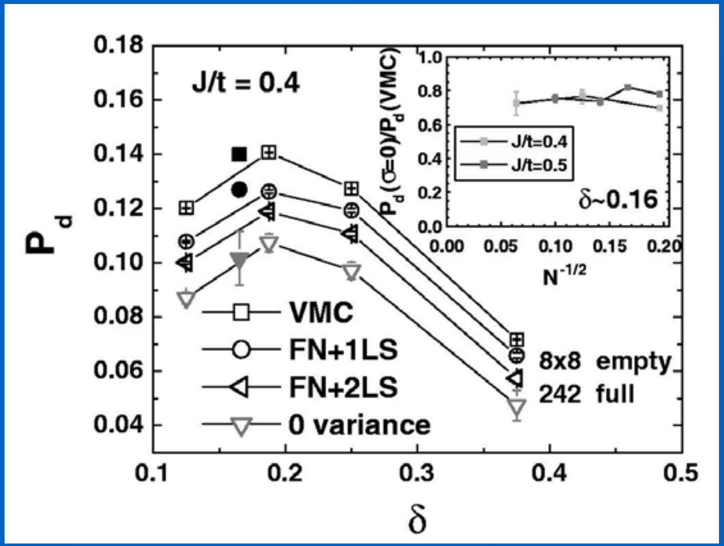
8-fold patterns
Bi2212

# Phase Diagrams of t-J Models for High-Tc

E.D., RMP 1994




Sorella et al., PRL 88, 117002 (2002)



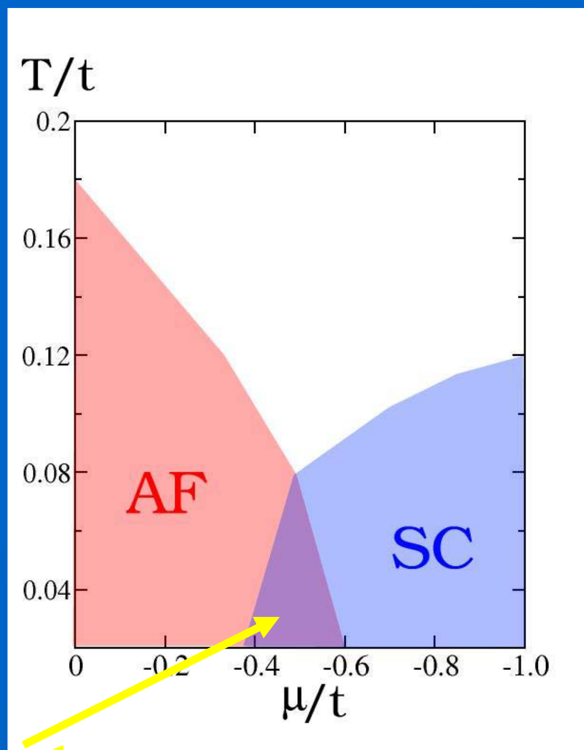

SC appears in simulations due to short-range AF, as in 2-leg ladders

Striped phase is close in energy

See PWA, cond-mat/0201429: ``The Cause is No Longer a Mystery''

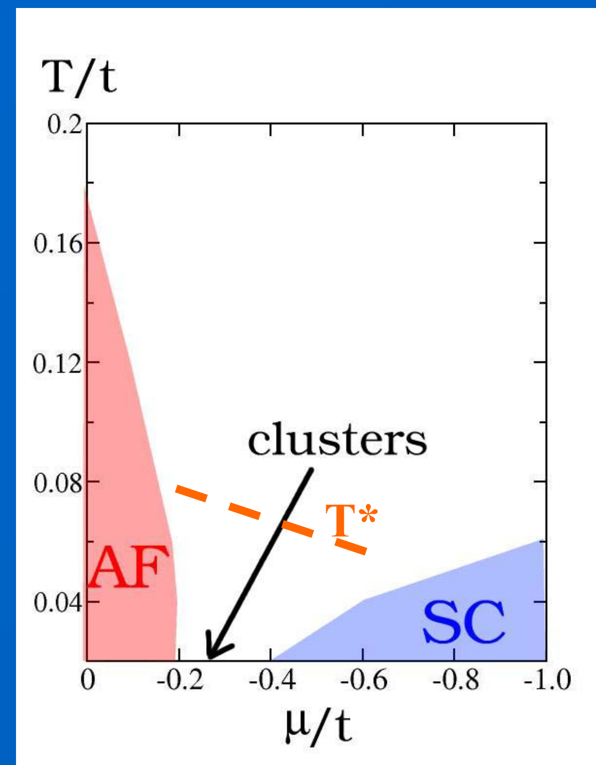
# In progress: SC vs. AF competition

**MC results for mean-field model of electrons coupled to classical AF** (Moreo et al., PRL 88, 187001 (2002)) **and SC order parameters** (Alvarez et al., in preparation)



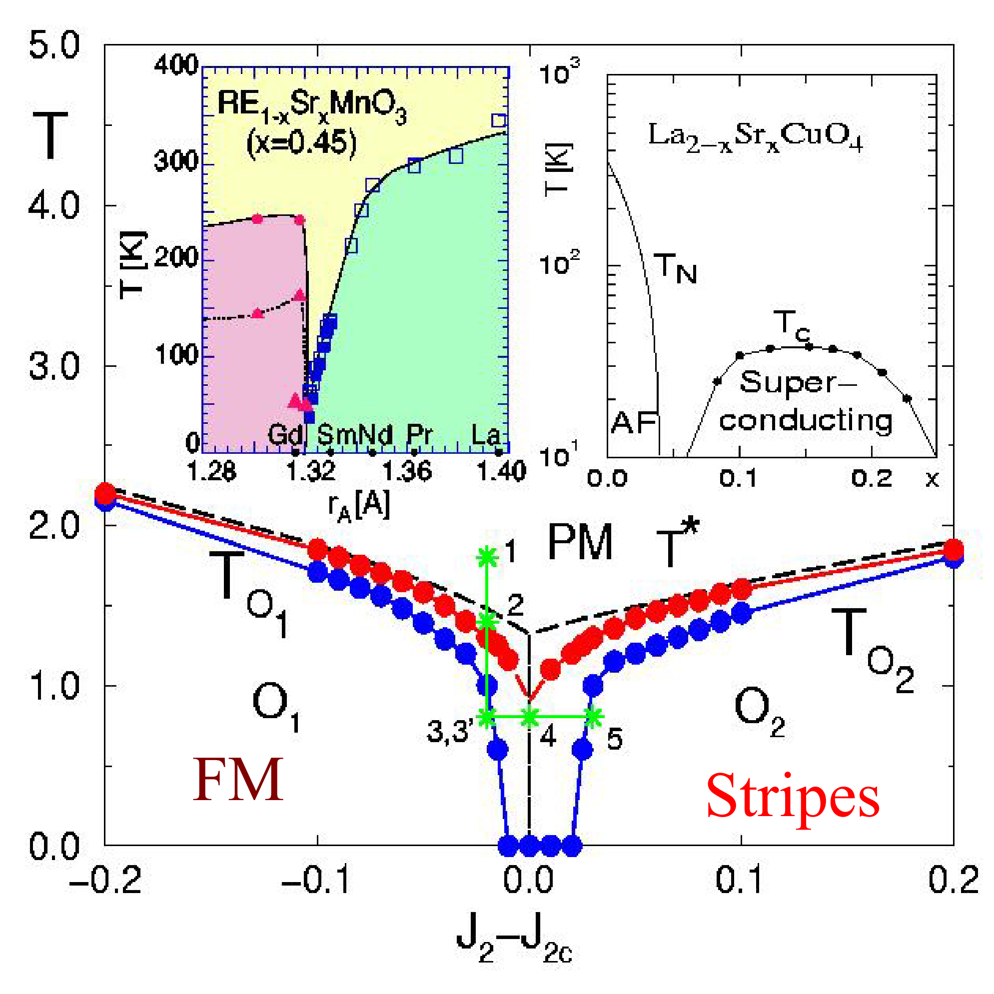

tetracritical

Without disorder

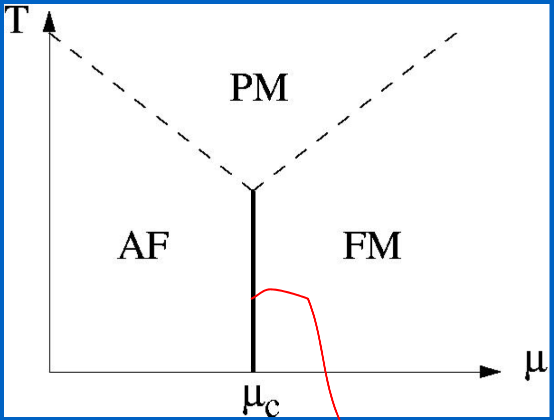



With Coulombic disorder

# Phase Competition in the Presence of Quenched Disorder




Previous result:



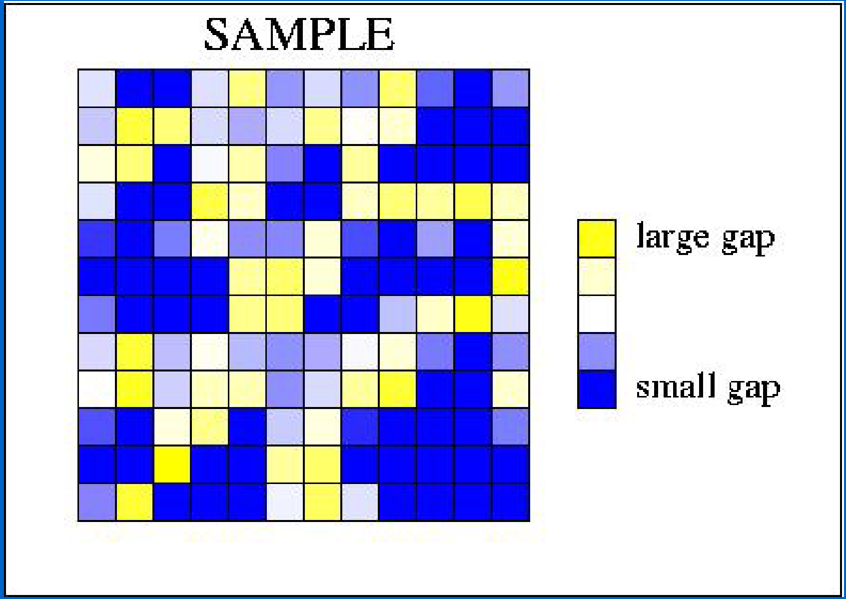

First order

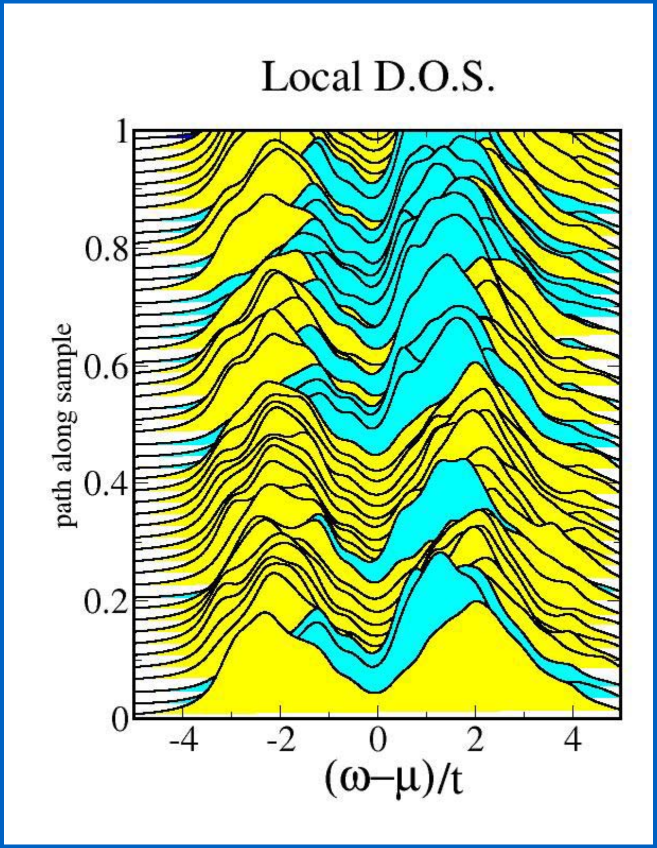
Toy Model with disorder

Burgy et al., PRL87, 277202 (2001).

See also Imry-Ma, Wortis,…

# Study of mean-field models including disorder (in preparation)

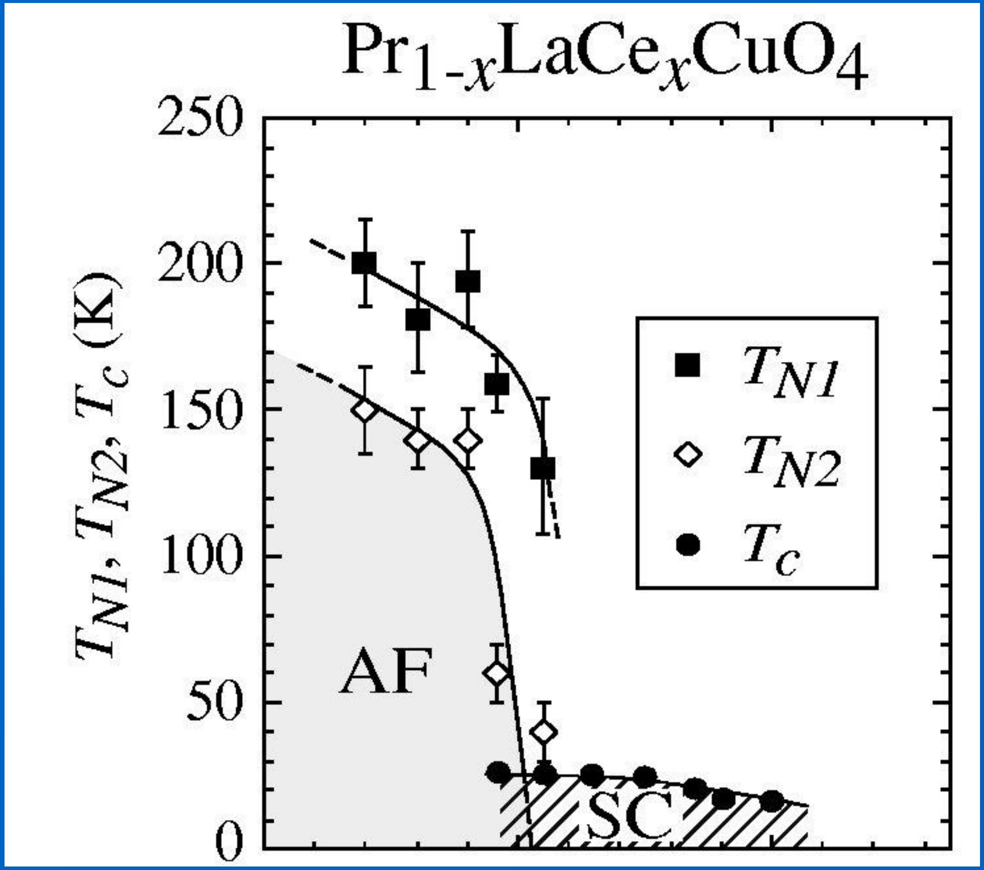



(see also DHLee et al. Wang et al.)

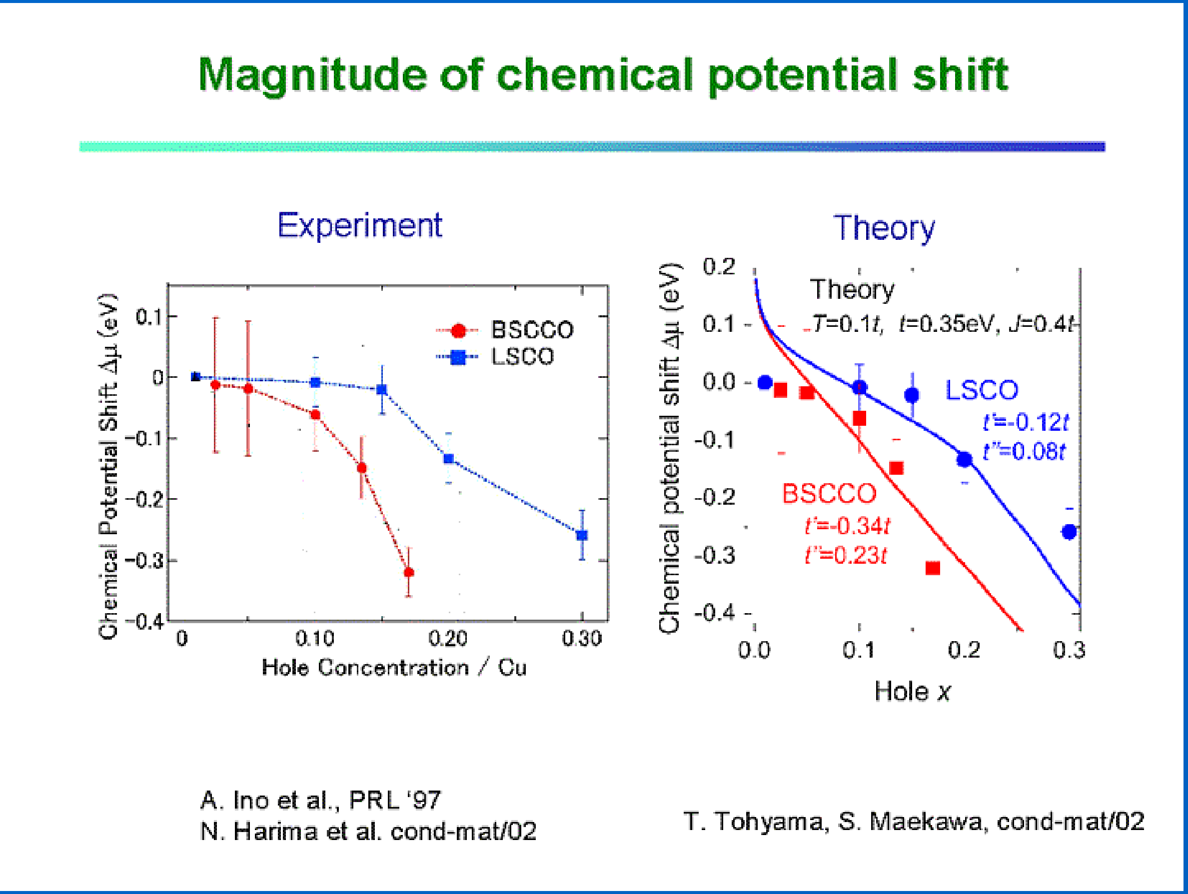
Large and small gap are caused by different local electronic densities caused by , e.g., randomly distributed Sr ions. Competition with AF in underdoped region is in progress.

# First-order SC—AF transition in electron-doped systems?




M. Fujita et al., cond-mat/0203320 muSR

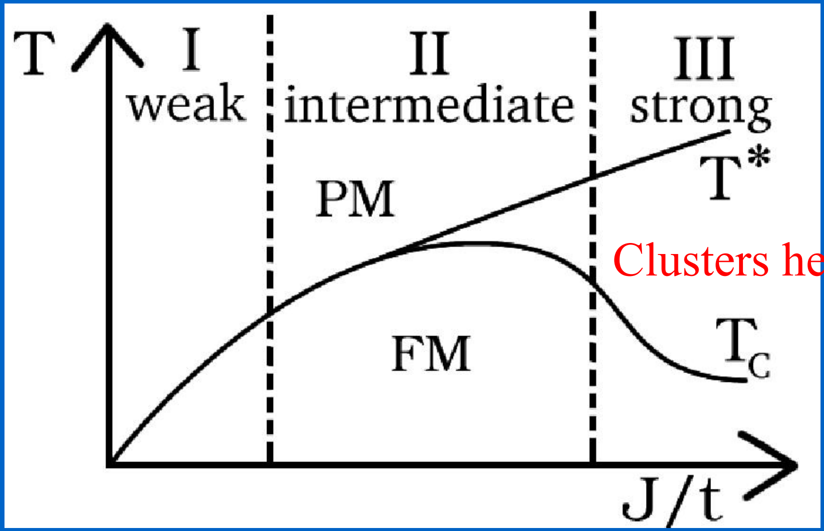
# Are stripes and inhomogeneities universal in cuprates?



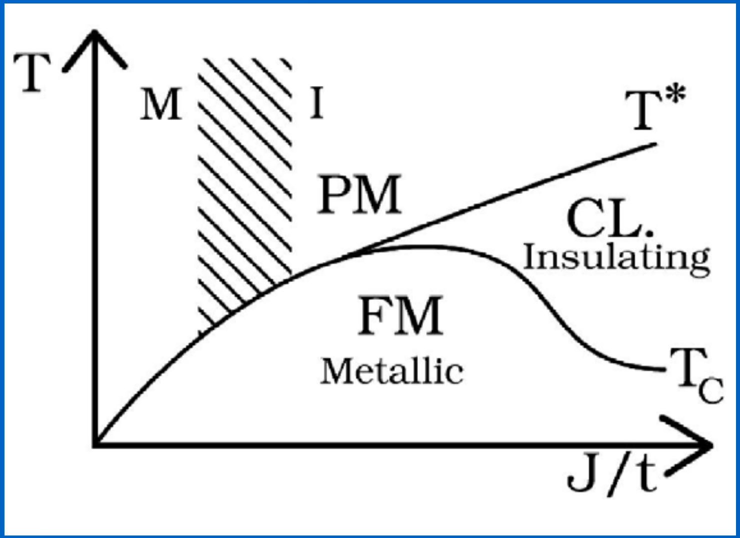

Att.: A. Fujimori
ITP conference
Nov. 2002

Some materials have tendencies to phase separate, but not all.

# Phase Diagrams (theory)




Clusters here

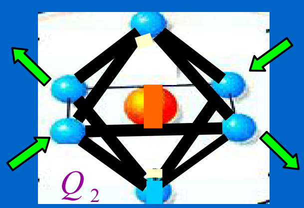



J is local AF coupling

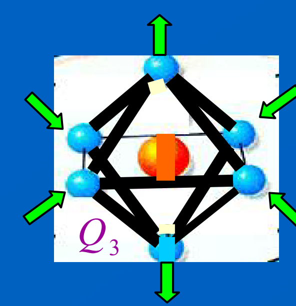
Mn spin < --- > carrier

# Two Orbitals plus Jahn-Teller phonons (Kanamori)

$$H = -\sum_{\langle i,j\rangle,a,b,\sigma} t_{ij}^{ab} c_{ia,\sigma}^{+} c_{jb,\sigma} - J_H \sum_{i,a,\sigma} S_i \cdot c_{ia,\sigma}^{+} \vec{\sigma}\, c_{ia,\sigma} +$$




$$+ g \sum_{i,a,\sigma} c_{ia,\sigma}^{+} Q^{ab}(i) c_{ib,\sigma} + \frac{k}{2} \sum_i tr\, Q^2(i)$$



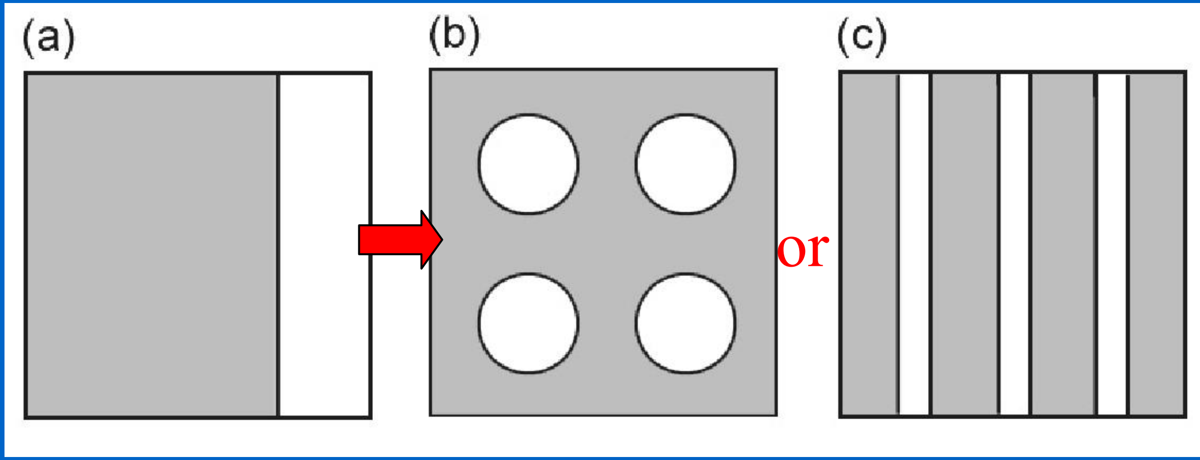

$$Q = \begin{pmatrix} Q_3 & Q_2 \\ Q_2 & -Q_3 \end{pmatrix}$$

g: electron-phonon coupling

k: phonon stiffness

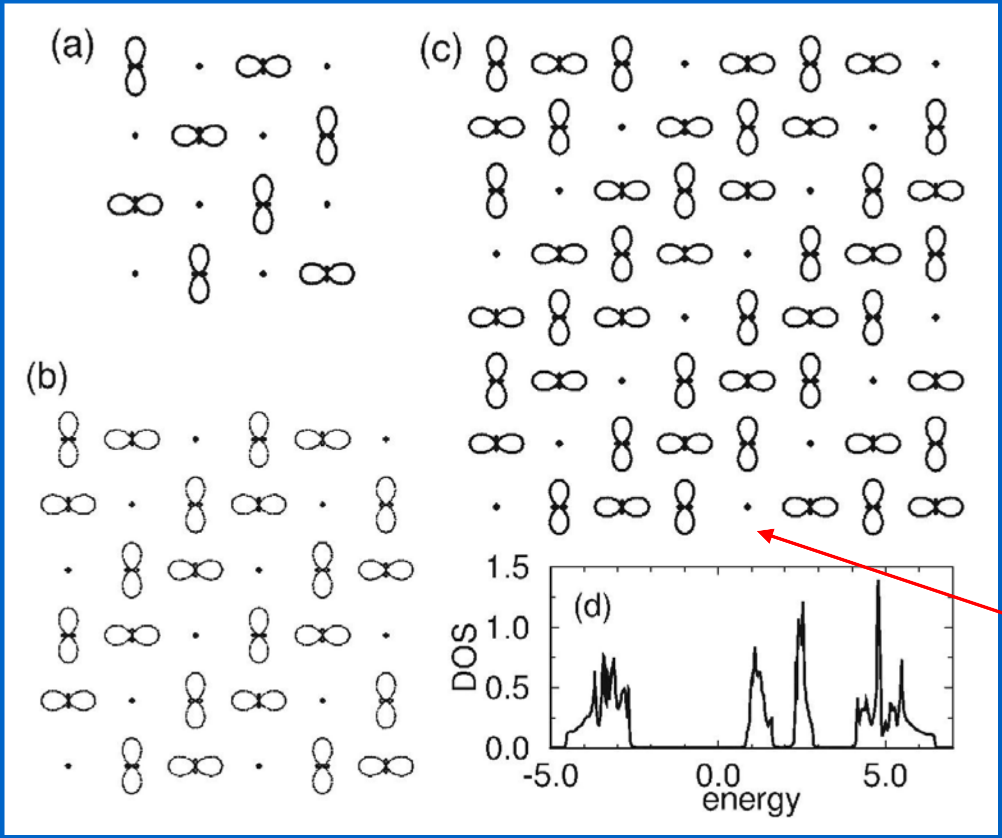
$\lambda = g / \sqrt{k}$

# Influence of 1/r Coulomb interaction




- Droplets, stripes or other nanometer size patterns may form (as in studies of high Tc and stripes, by many authors).
- In 1D the PS state evolved into CDW state with increasing repulsion (Malvezzi et al. PRB '99).

# Stripes exist as the ground state at large e-JT coupling



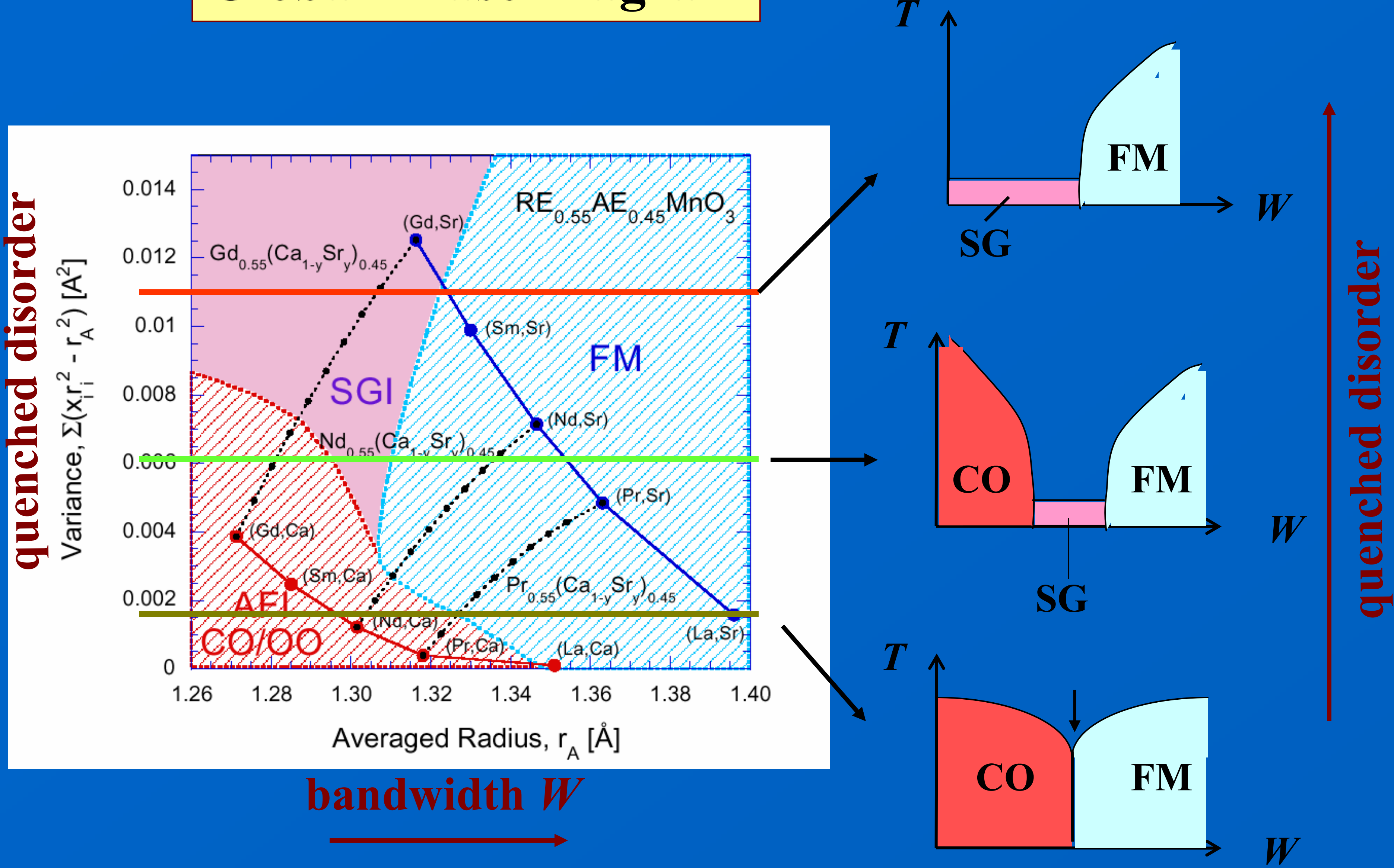

Ferromagnetic phase.

Hotta et al.
PRL86, 4922 (2001)

More about new phases later!

Pi-shift in orbital order. 1/r not needed.

# Global Phase Diagram




Courtesy: Prof. Yoshi Tokura, Tokyo.

# Computational Techniques

- Partition Function

phonons $t_{2g}$ spins

$$Z = \int DQ \int DS \, \overbrace{tr_{e_g}\left(e^{-\beta H}\right)}^{e_g \text{ electrons}}$$

$$S_i = \left(\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i\right)$$

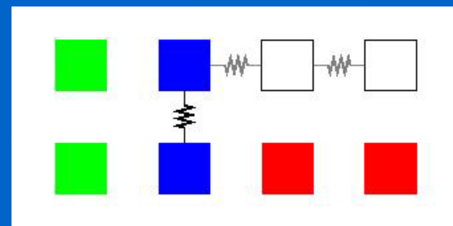
•Monte Carlo simulation over classical spins. Quantum itinerant electrons treated exactly.

•No sign problems. All temperatures and densities are accessible.

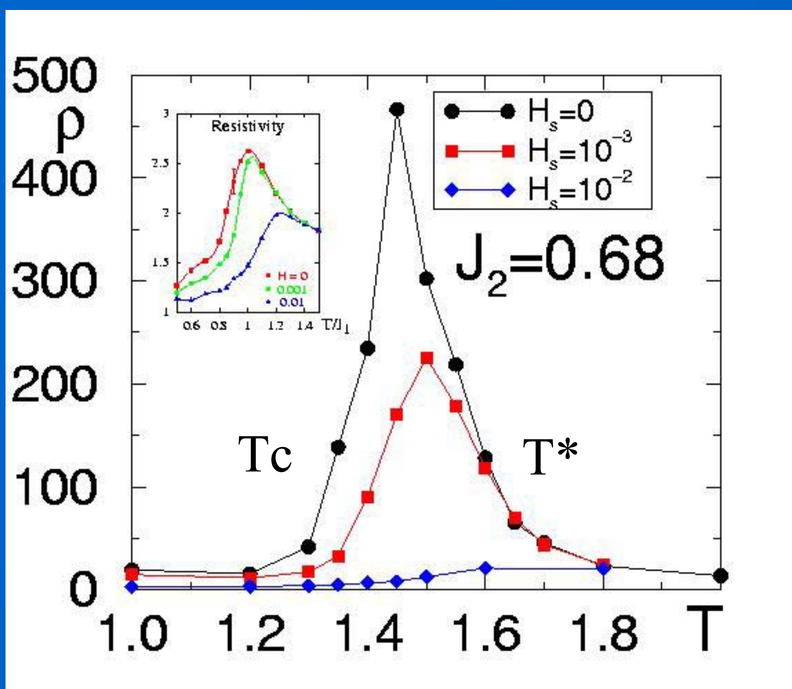
•Classical approximation tested in 1D comparing with Lanczos.

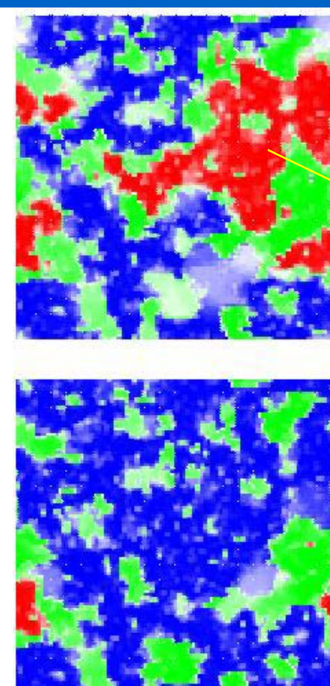
•Dynamical properties can be calculated straightforwardly.

# CMR effect in inhomogeneous states



Resistor Network: FM up FM down Insulator Disorder



H=0

Rotates easily

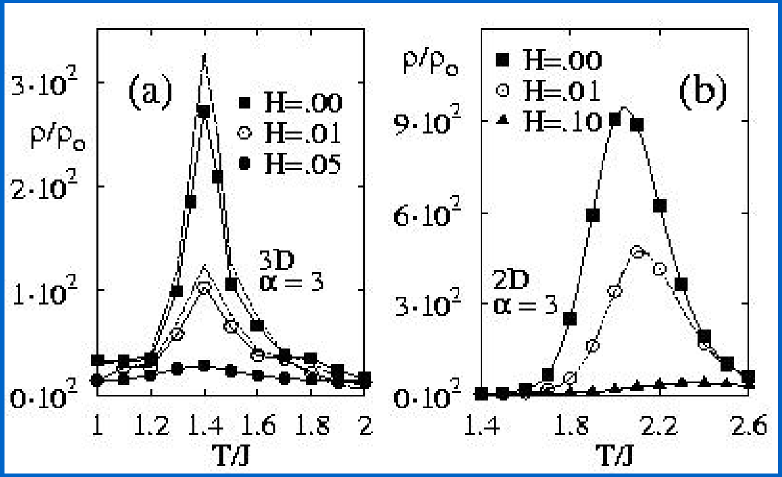
Field is small, but effective spin is large!

H=0.01

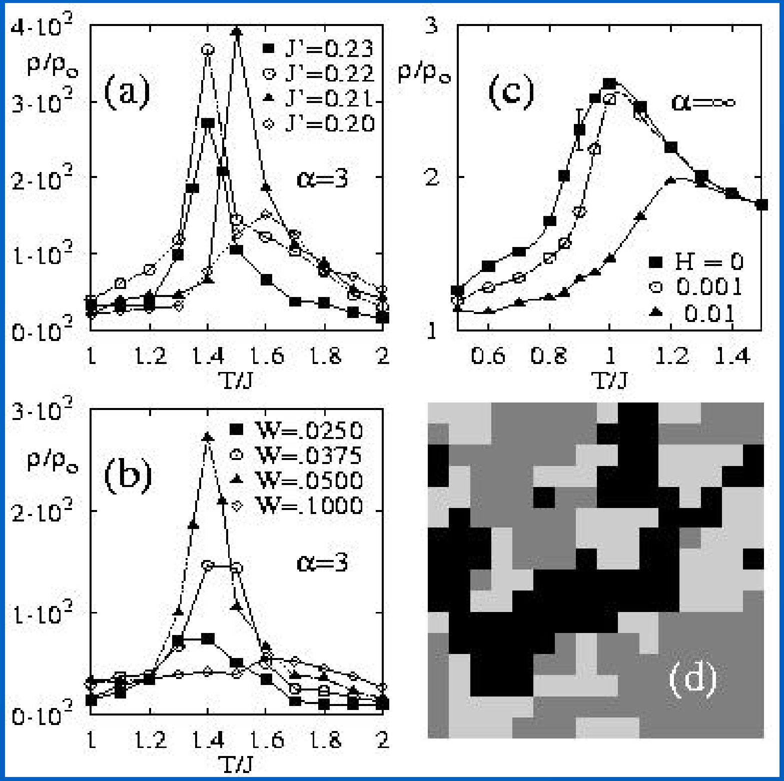
MR ratios as large as 1000% at H=0.01 (PRL 87, 277202 (2001)).

# Resistivity with correlated disorder

3D 2D

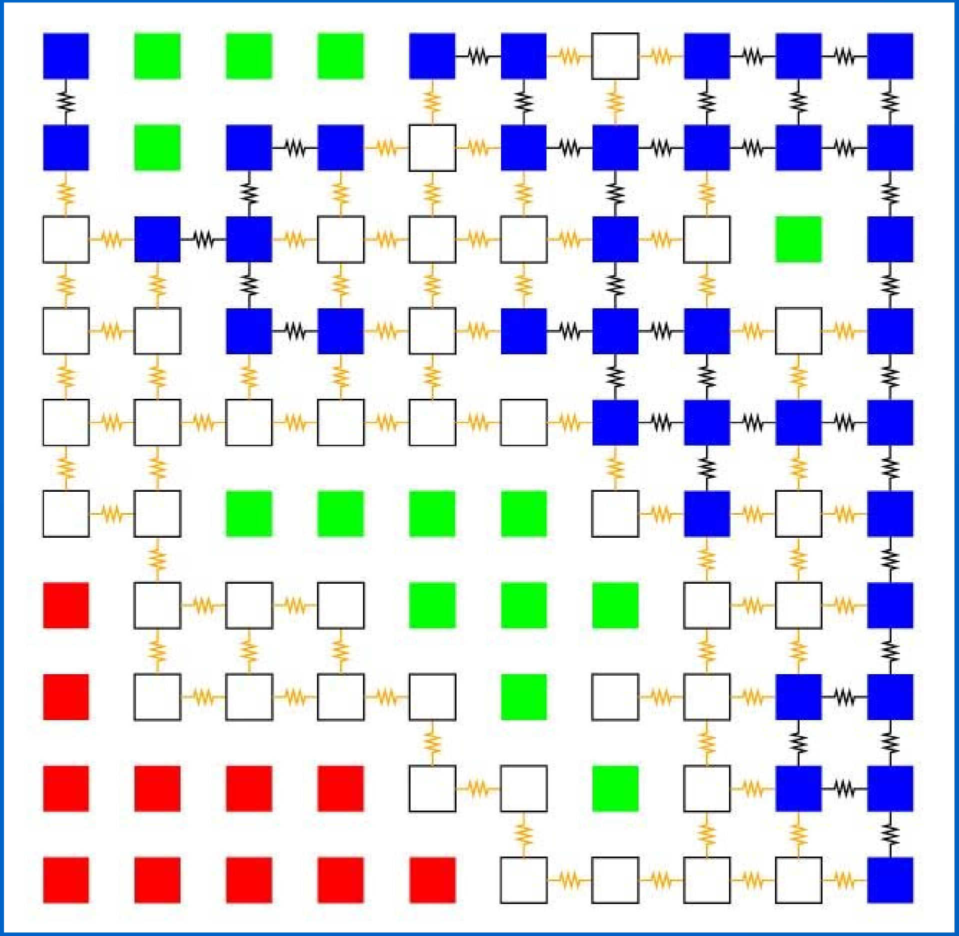



J1-J2 model. Now 3D and 2D are very similar!

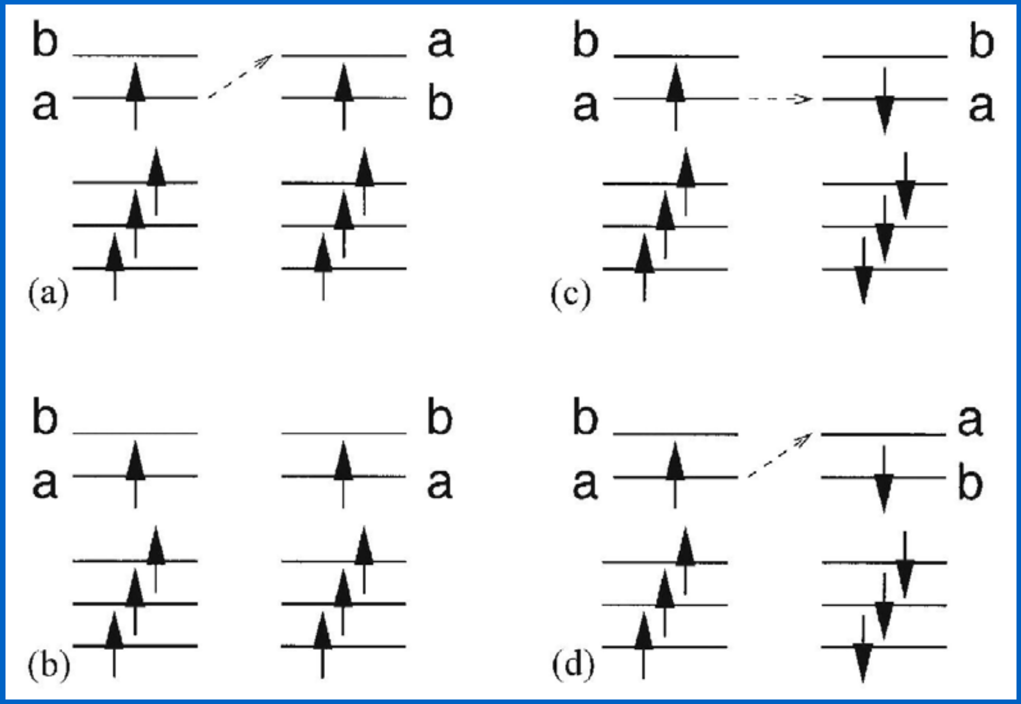



Cluster shapes in 3D.

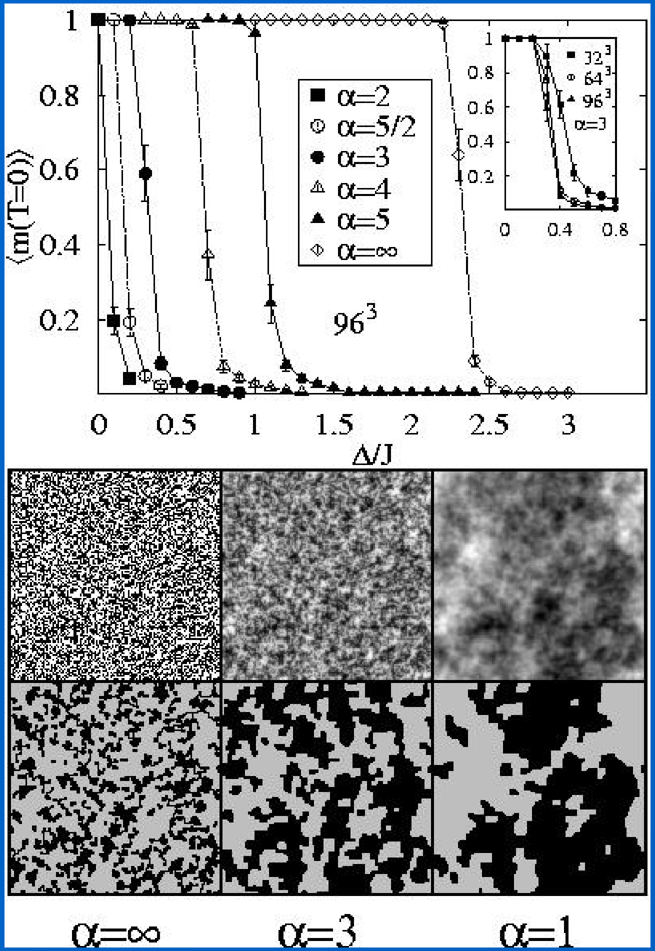
# Random Resistor Network



# Staggered Orbital / FM



# Random-field Ising Model with Correlated Disorder

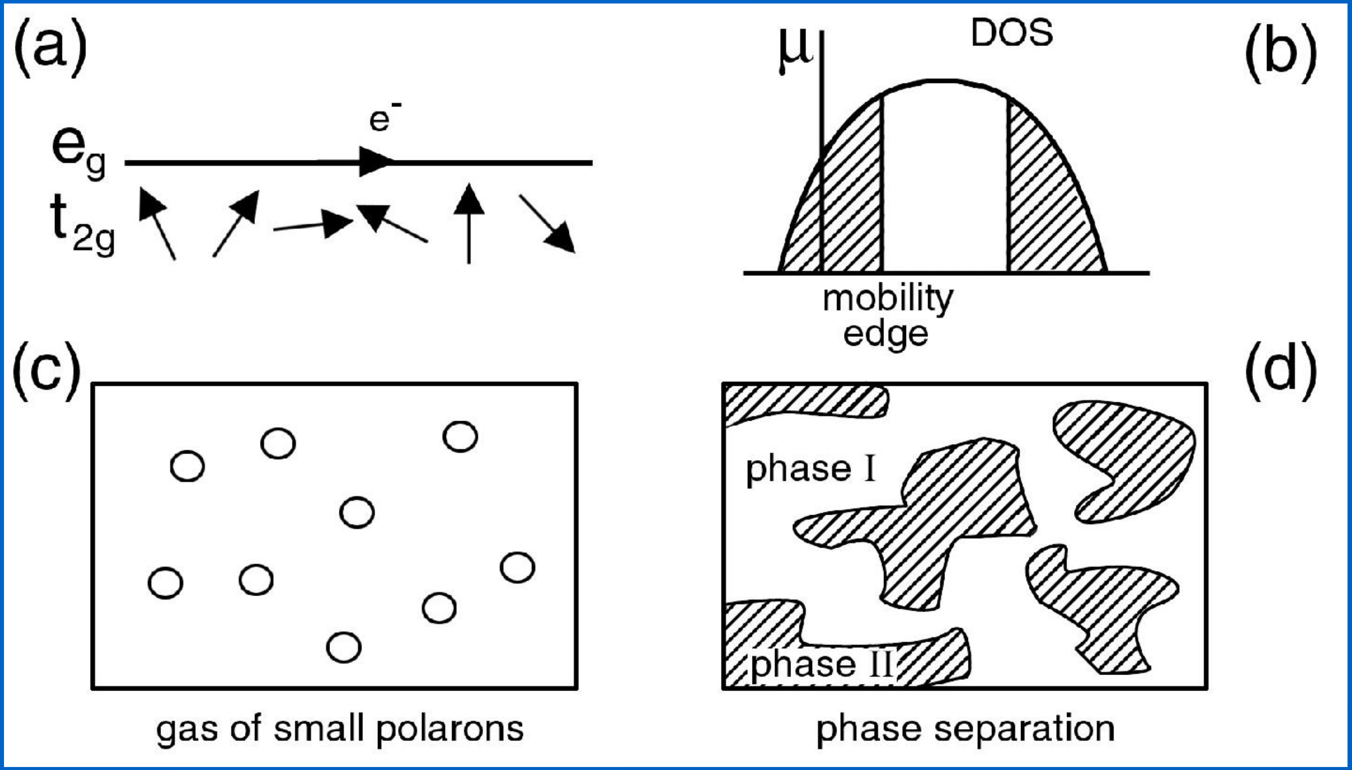



T=0 magnetization vs. strength of disorder. Drastic reduction of critical Delta by disorder correlation.

Disorder distribution

Clusters

# Possible theories of CMR



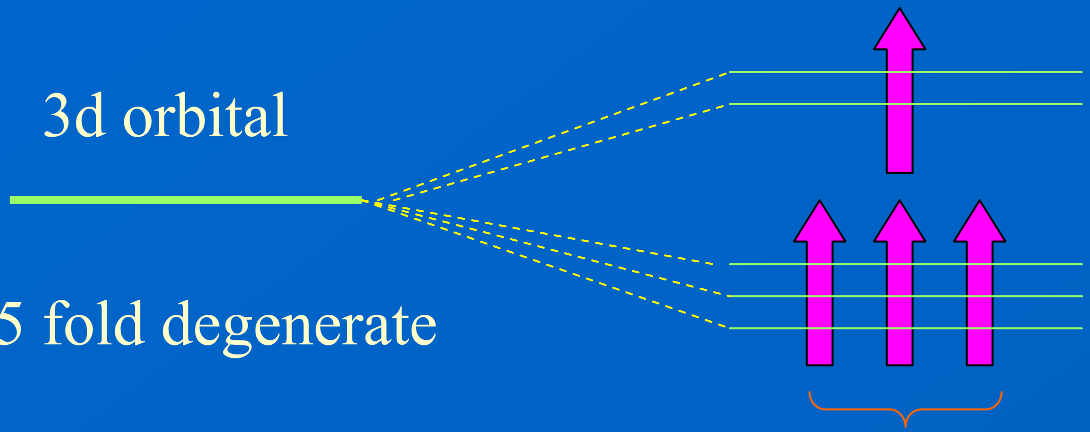

This talk

# Models for Manganites

$Mn:[Ar]3d^5 4s^2$

$Mn^{3+}:[Ar]3d^4$

3d orbital



5 fold degenerate

$e_g\left(d_{x^2-y^2}, d_{r^2-3z^2}\right)$

$t_{2g}\left(d_{xy}, d_{yz}, d_{zx}\right)$

S=3/2 (localized)

# The Lattice Kondo Model

## 1 orbital approximation

$$H = -t\sum_{\langle i,j\rangle}\left(c^{+}_{i,\sigma}c_{j,\sigma} + c^{+}_{j,\sigma}c_{i,\sigma}\right) + J\sum_{i} s_i \cdot S_i + J_{AF}\sum_{\langle i,j\rangle} S_i \cdot S_j$$

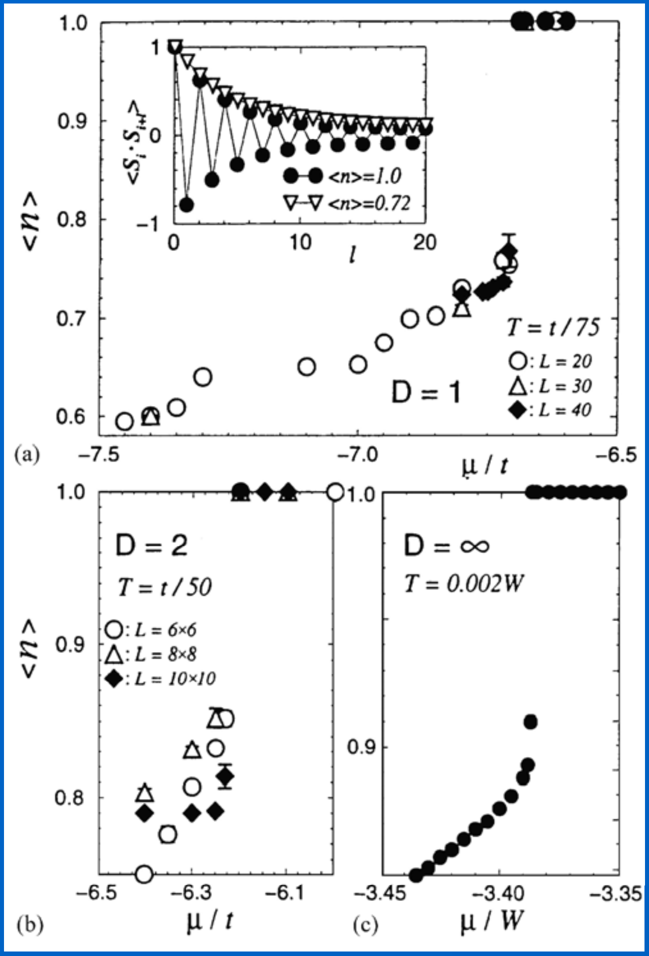
Heavy Fermions: J/t<<1

Manganites: |J/t|>8, J<0

J/t

A. Moreo et al.,
Cuprates: J/t~2
PRL84, 2690 (2000)

# Monte Carlo and DMFT evidence of phase separation in 1-orbital model

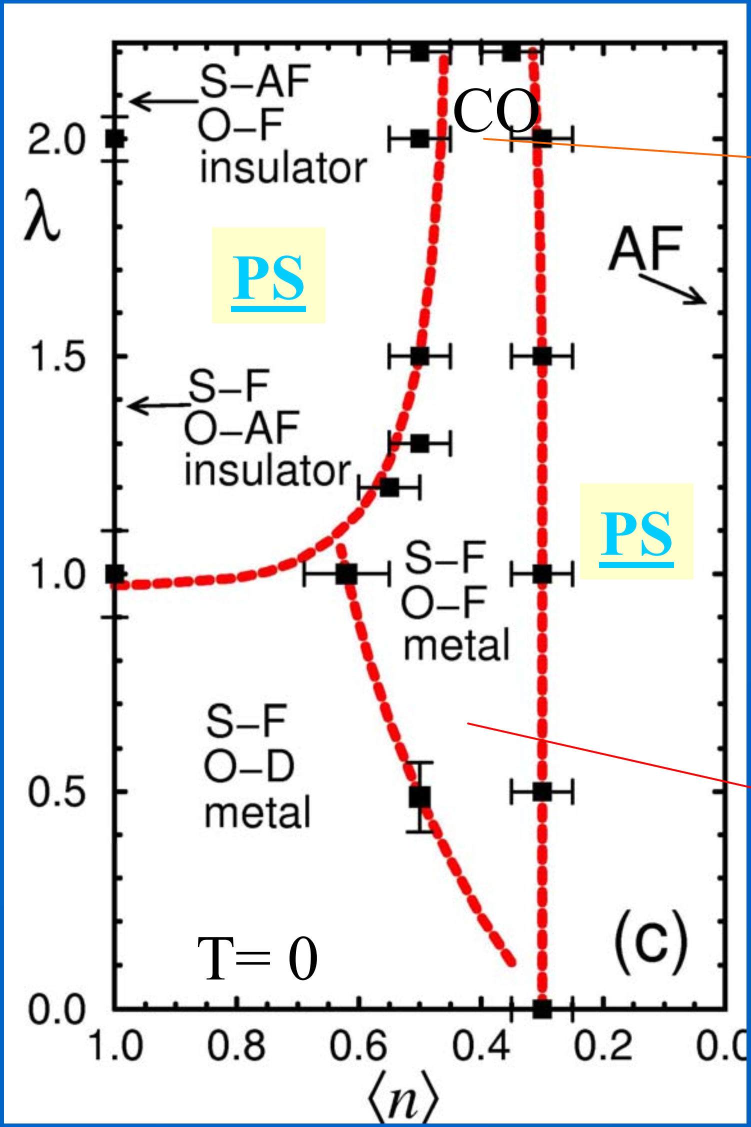



Phase separation manifests as a discontinuity in density vs. chemical potential.
It appears in all dimensions investigated .

Yunoki, Furukawa, et al., PRL 98. See also Guinea, Arovas, …

Similar in spirit to the phase separation found in the t-J model, although there it involves SC and AF.

# 2 Orbitals and J-T Phonons



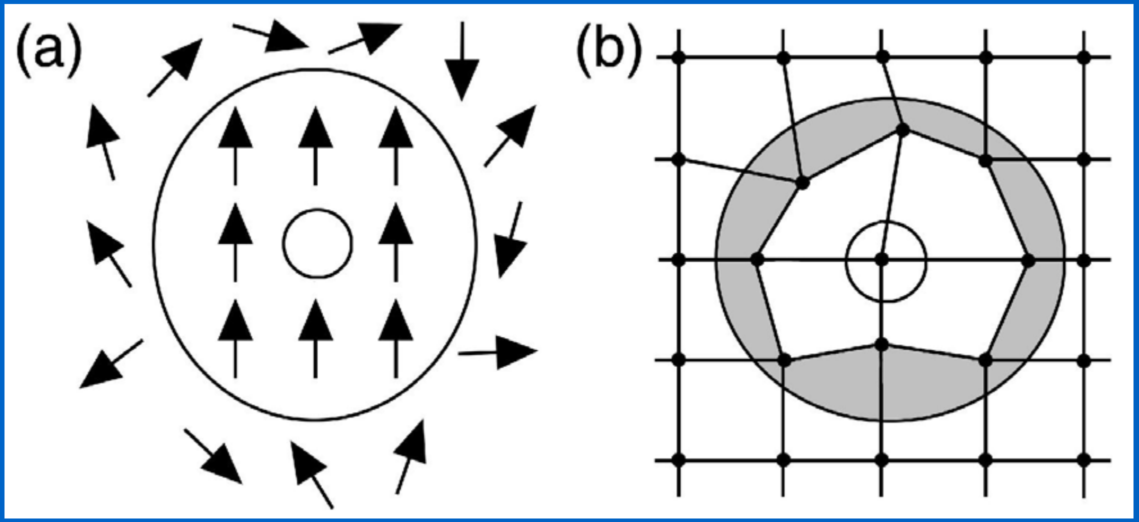

Precursor of CE

- All the stable phases observed experimentally are obtained.
- PS very prominent as in 1 orbital model.

Precursor of A-type AF

Yunoki et al.,
PRL 81, 5612 (1998)

# Polarons or Larger Clusters?

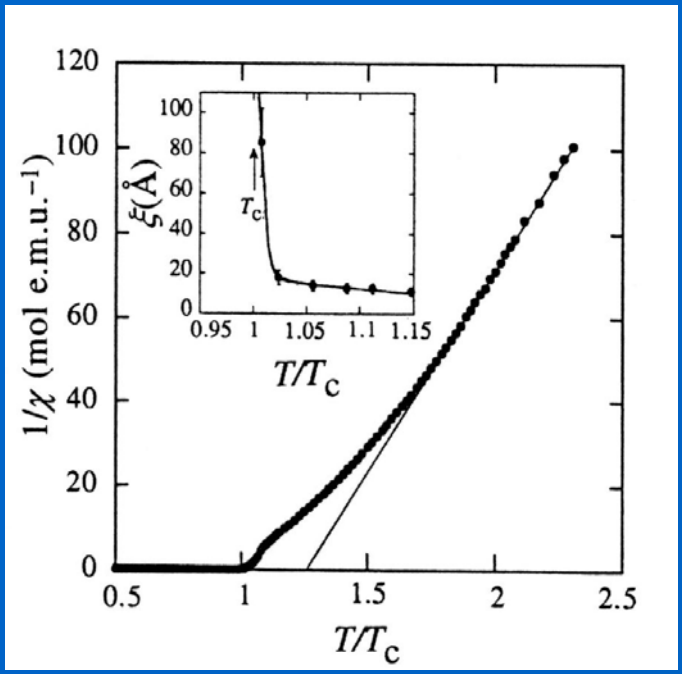



FM Polaron                Lattice polaron

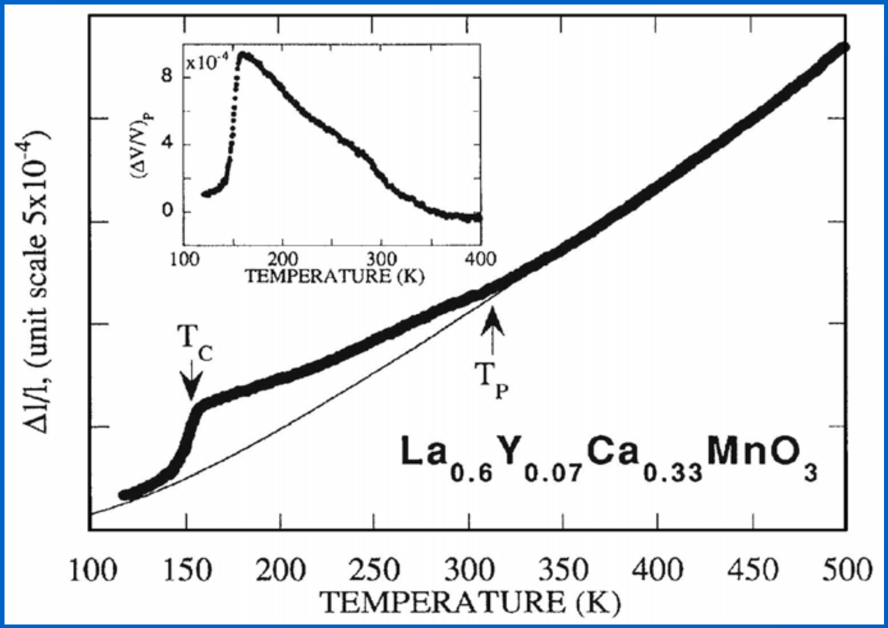
One carrier surrounded by a distortion.

Mn oxide experiments reveal far larger clusters, with many carriers inside. Polaron picture not suitable.

# Additional evidence of T*



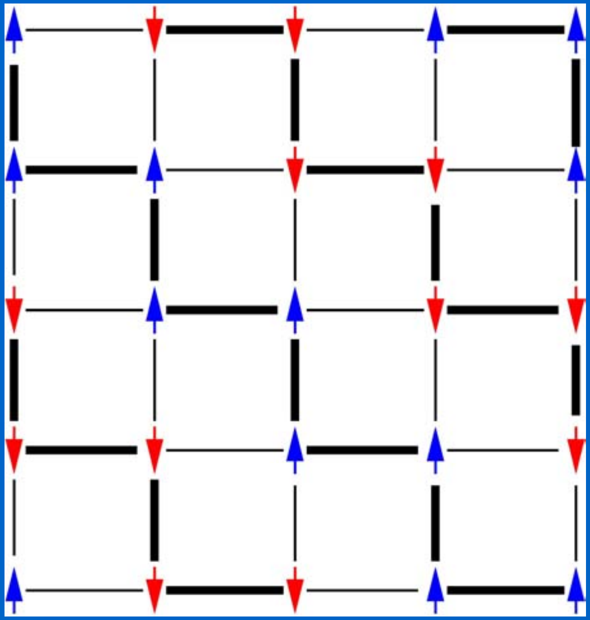

LCMO

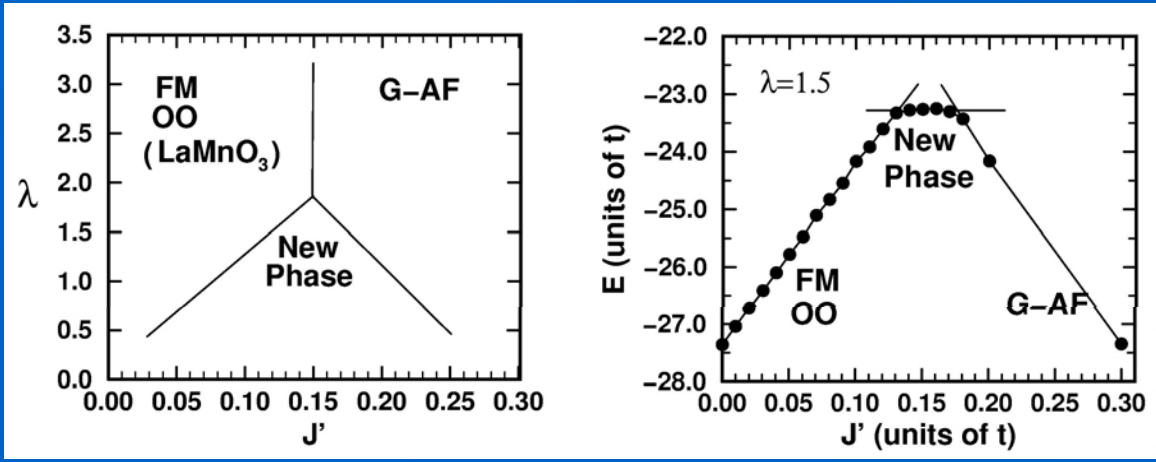



Thermal expansion

From De Teresa, Ibarra et al.

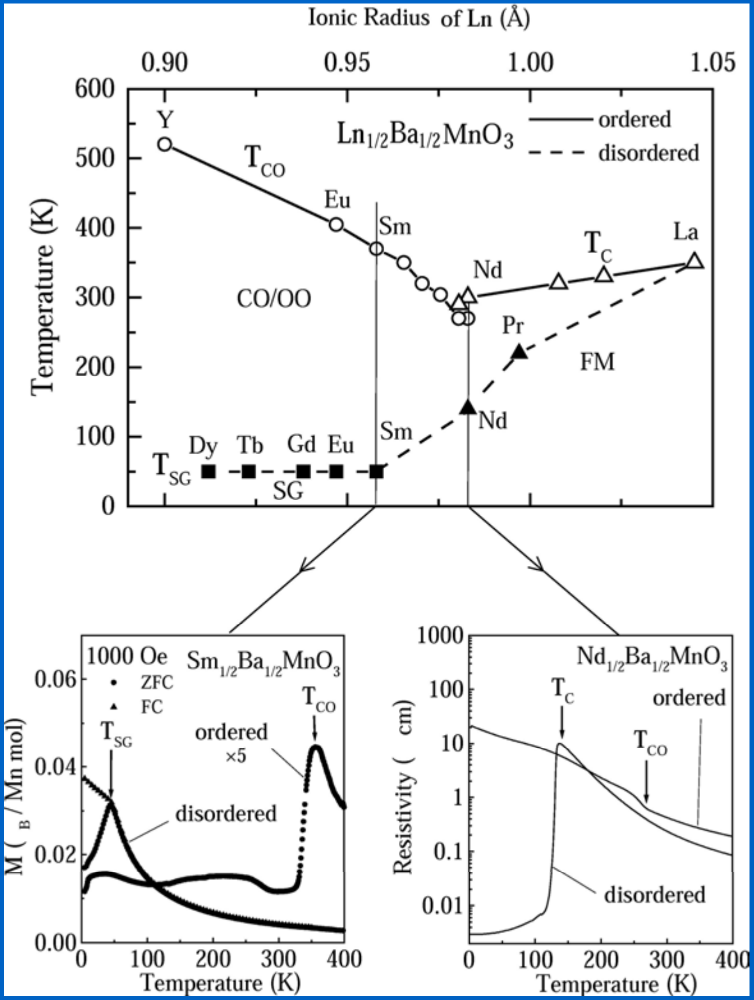
# Very recent developments: New ``E-phase'' in undoped limit






Hotta et al., cond-mat
See also Kimura et al.
(experiments).

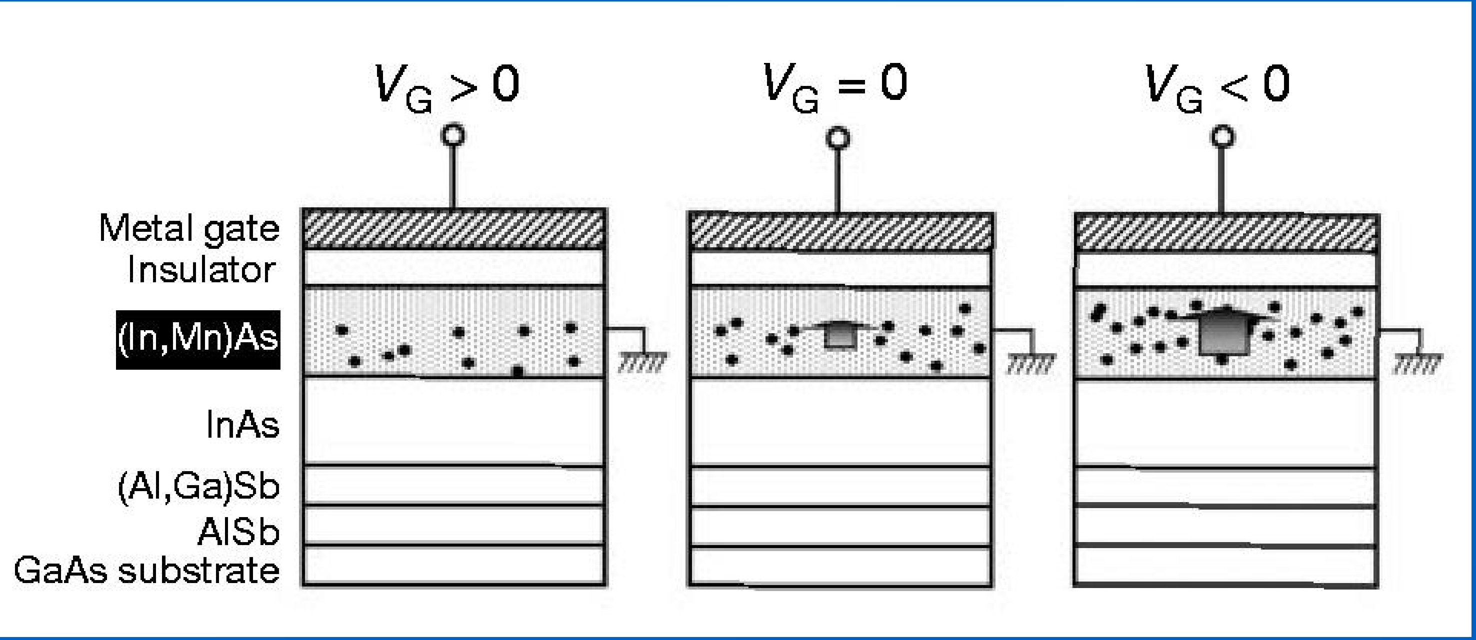
# Experimental phase diagrams with and without disorder



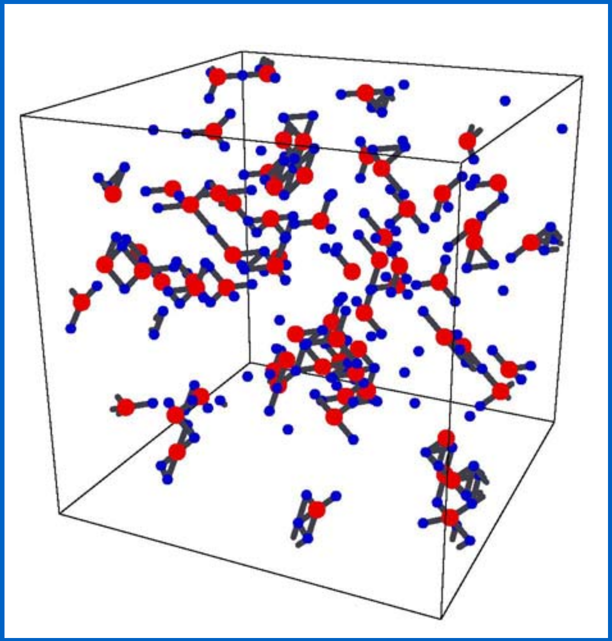

Dramatic changes with and without disorder. CO phase affected the most.

Tokura, Ueda, et al., 2002

# Spin-polarized field-effect transistor (I)



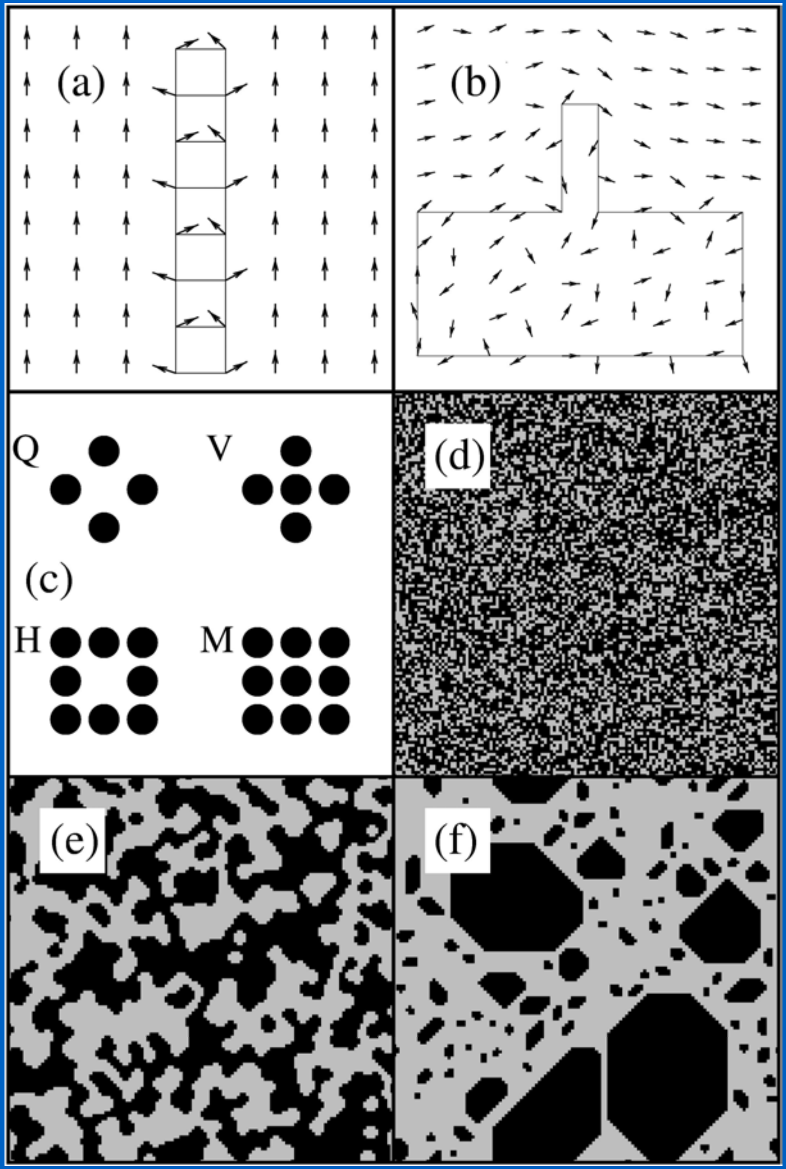
# Other evidence of clustering



Timm et al.,
PRL
Origin: Coulomb
repulsion

Rounded clusters mimic better the surface tension effects.

First-order percolation observed in some models (Burgy et al., PRB 03)

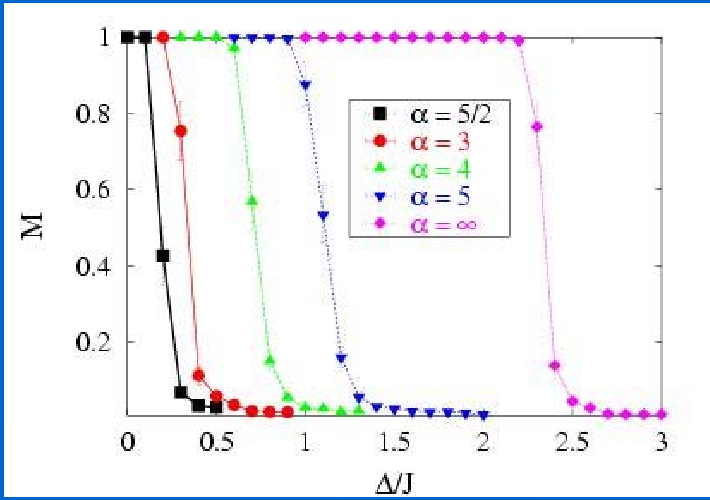



Standard percolation

Metal vs. insulator character determined based on neighbors

# New: Correlated disorder

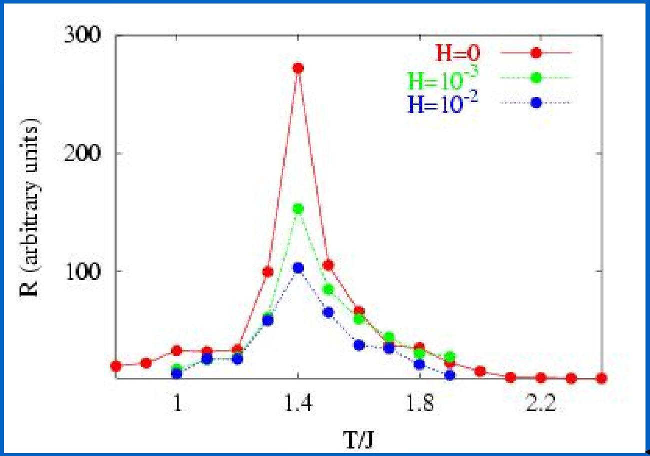
(Idea: each doped element distorts a finite region around)




Dc=3 for
Alpha<2.5

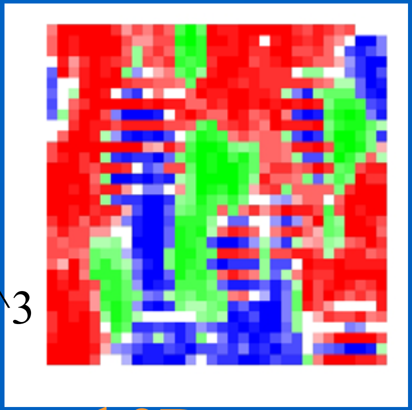
64^3 cluster

Random Field Ising
Model with power-law
correlated disorder




3D
alpha=3
16^3

J1-J2

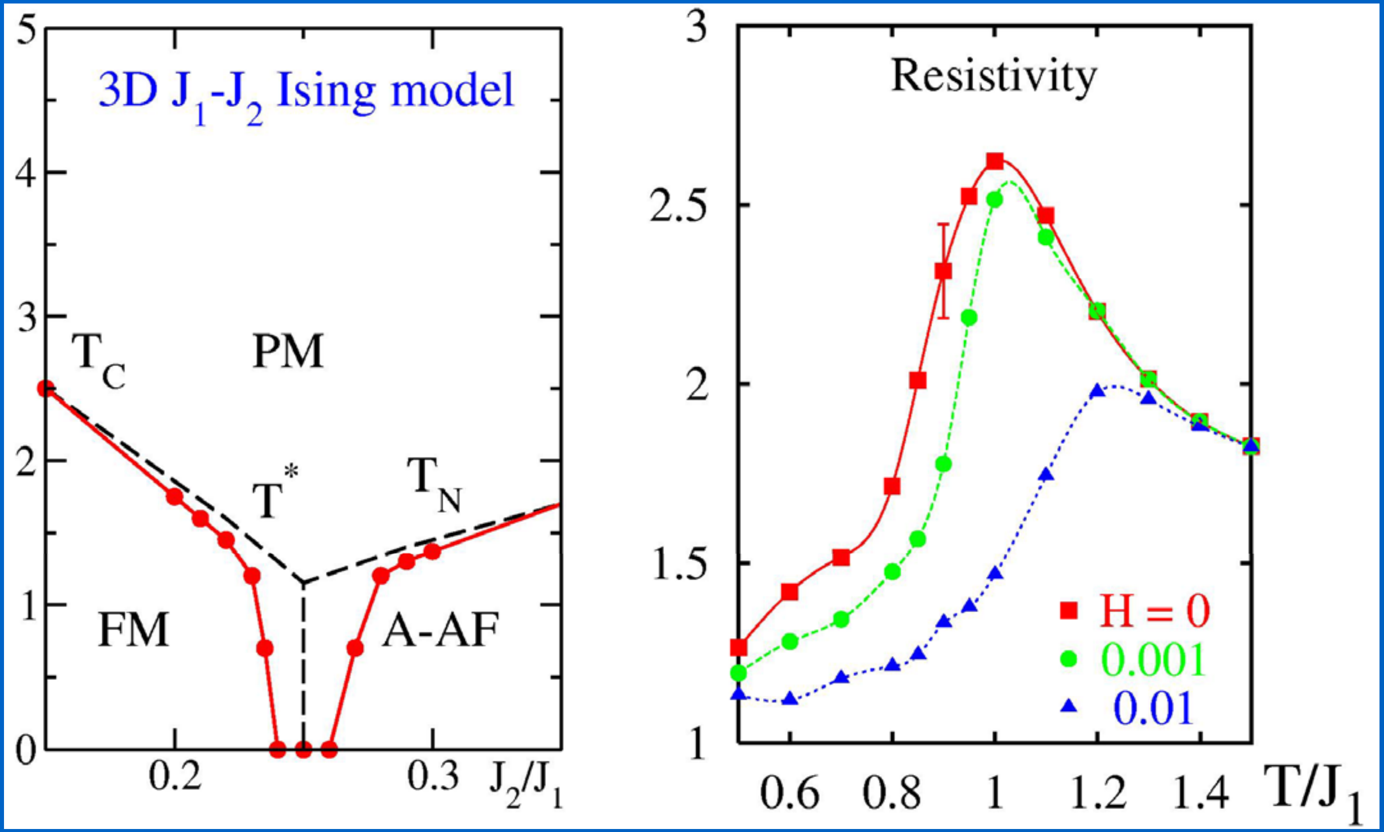


64^3

Spin up
Spin down
Insulator

3D and 2D are now similar

# Similar results in 3D

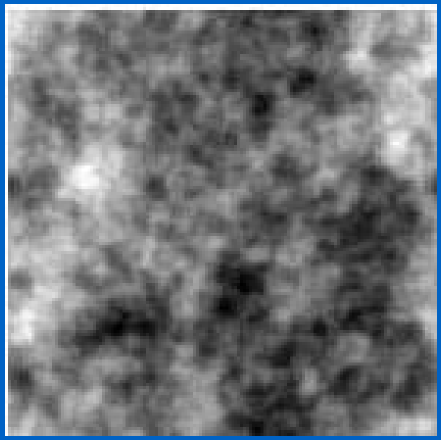



Qualitatively as in experiments, but with smaller intensity than in 2D..
Are longer range interactions needed? (strain, Coulomb)

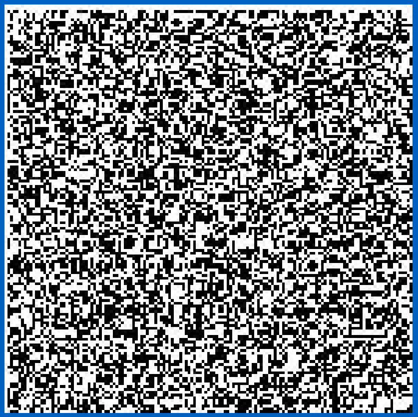
# Cluster shapes with correlated disorder

128 x 128

Alpha = 0.1



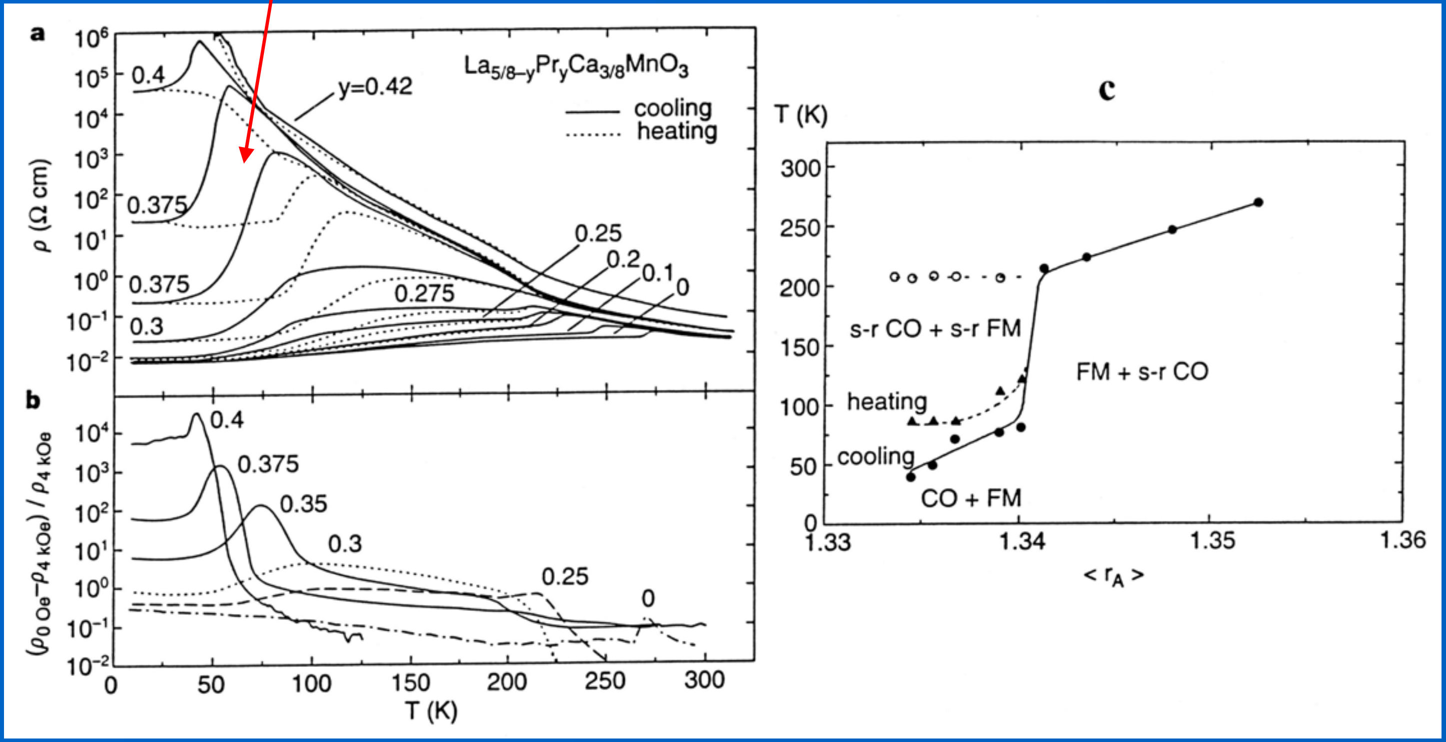
1.0



oo (short-range)

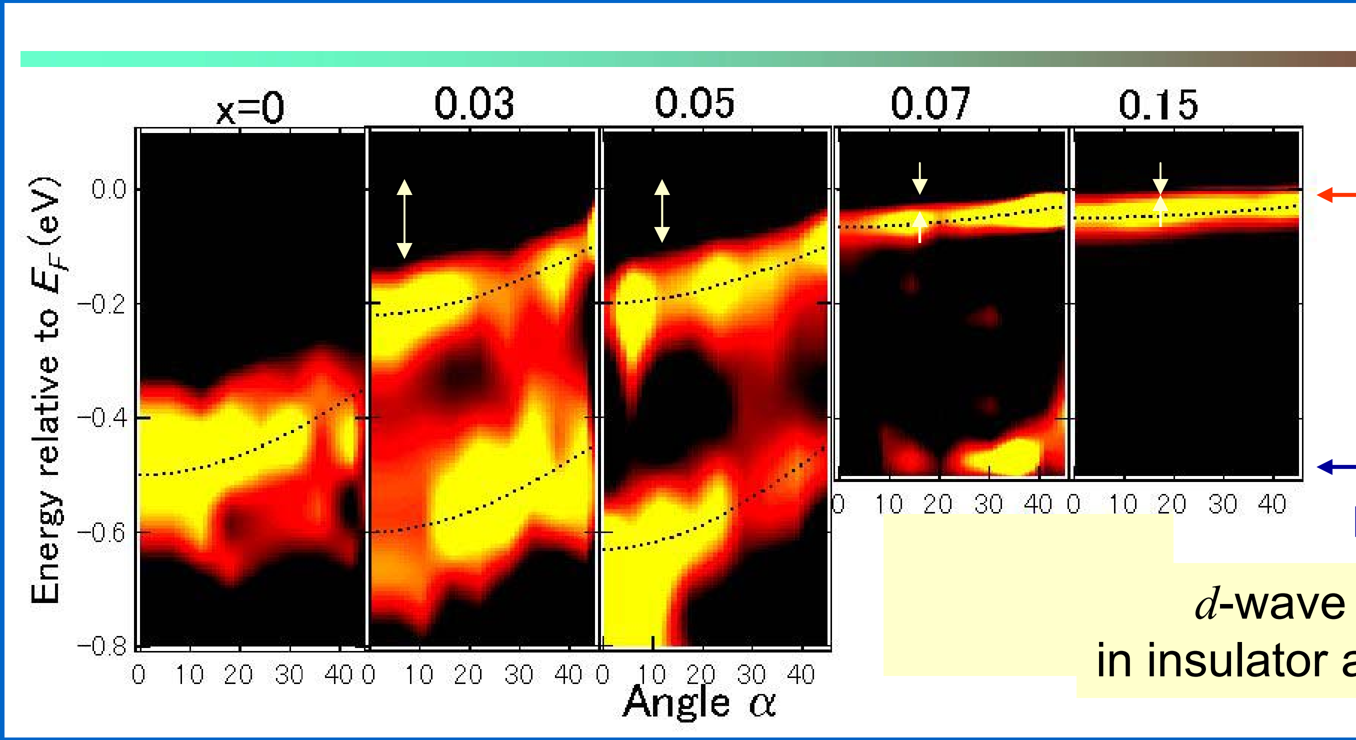
# Unsolved issues: First-order/percolative mixture?

Percolative “and” first-order ?




Uehara et al., Nature 1999

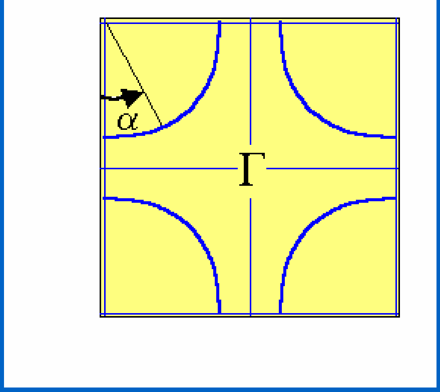
# Dispersion along Fermi surface in $La_{2-x}Sr_xCuO_4$



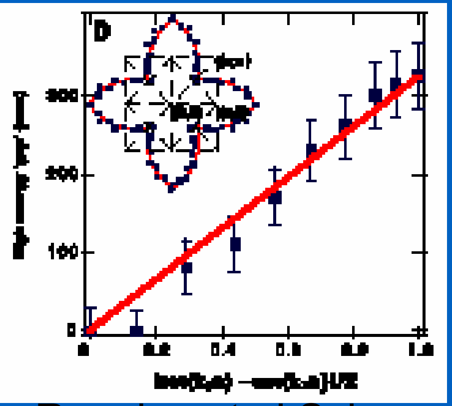

"In-gap" states with superconducting gap or normal-state gap

lower Hubbard band

$d$-wave like anisotropy
in insulator and superconductor




$Sr_2CuCl_2O_2$




Ronning et al.Science '98

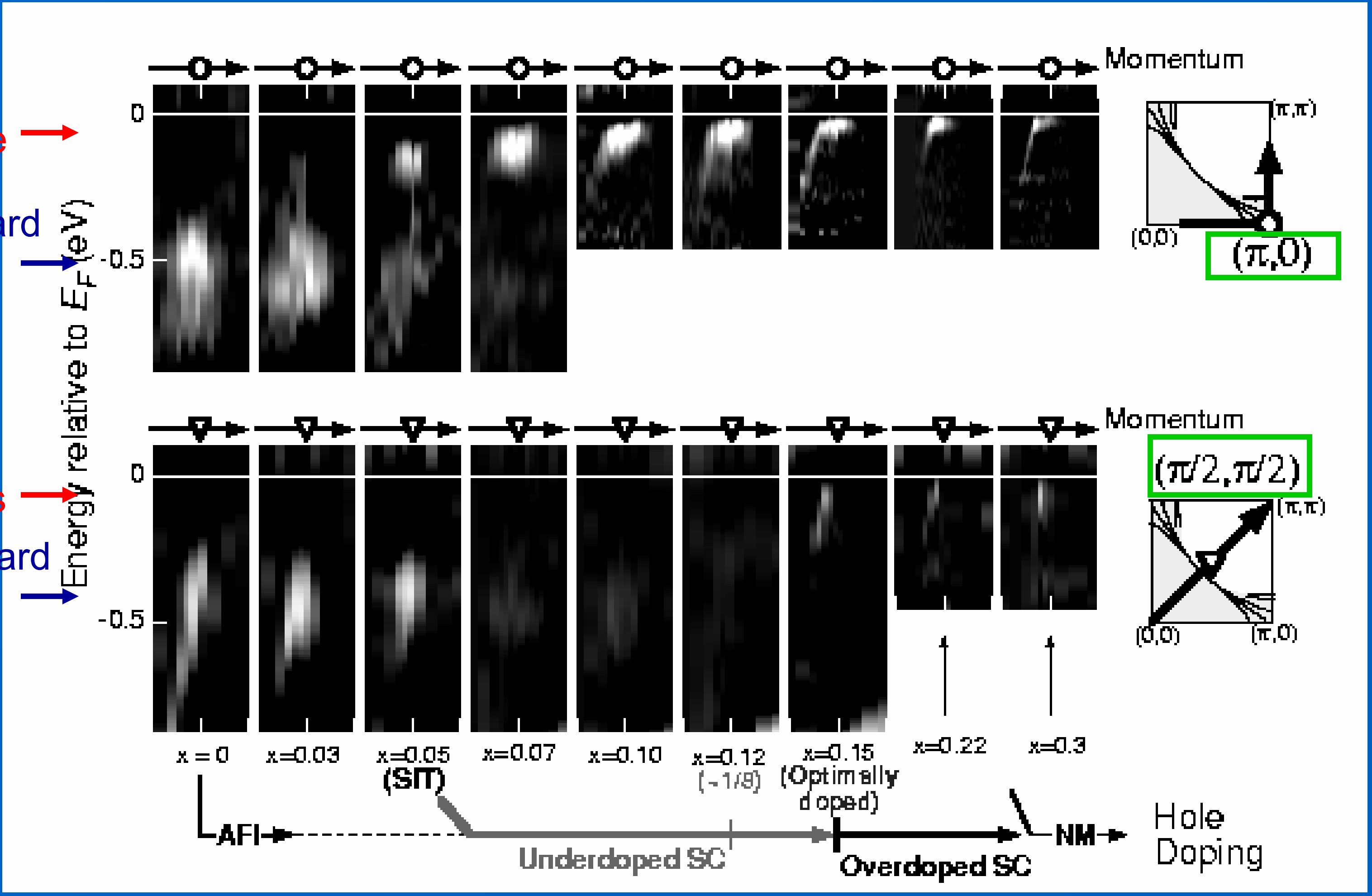
# Two-component electronic structure in underdoped $La_{2-x}Sr_xCuO_4$

Flat band/ ($\pi$,0) feature

Lower Hubbard band

Nodal states

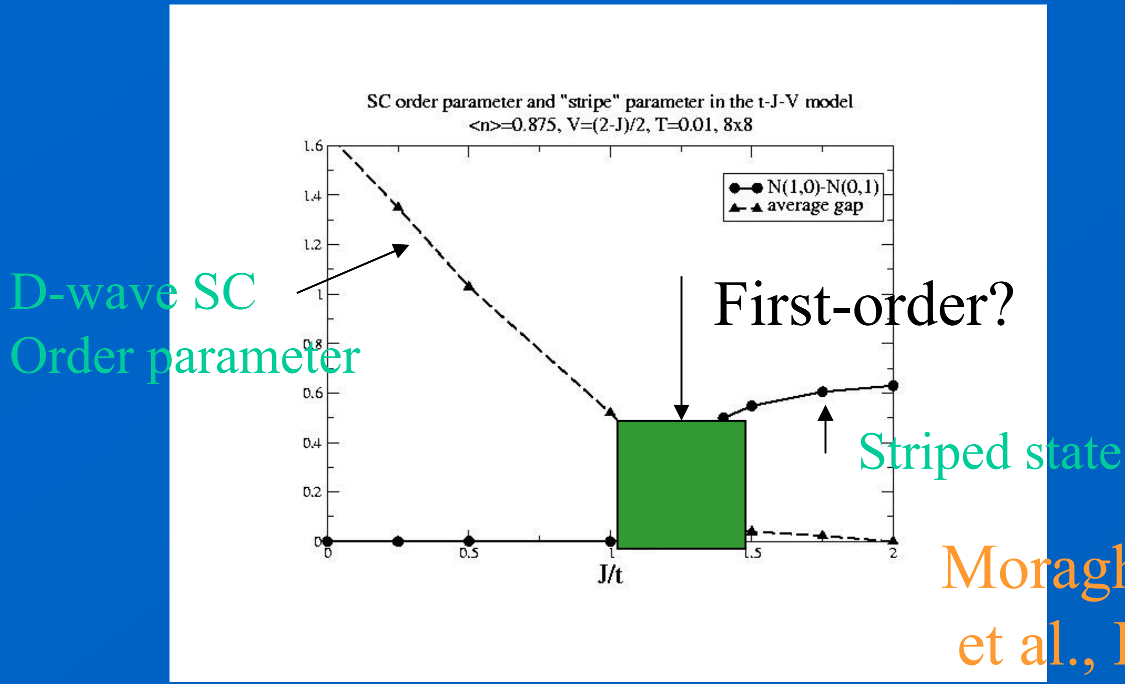
Lower Hubbard band




Ino et al., PRB '02

# New: SC vs. Stripes simulations

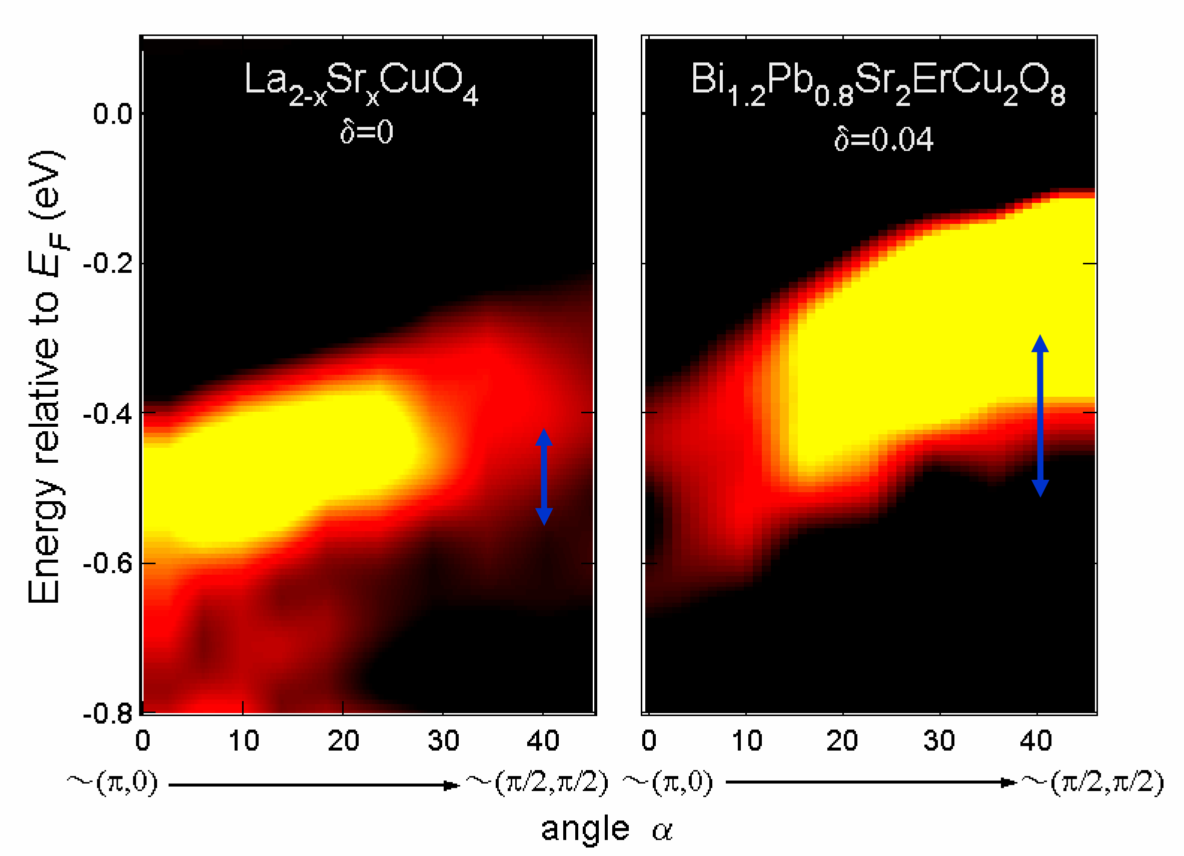
Toy model: fermions interacting with classical local spins and classical complex d-wave SC order parameter. Phase diagram has SC and Striped phases.

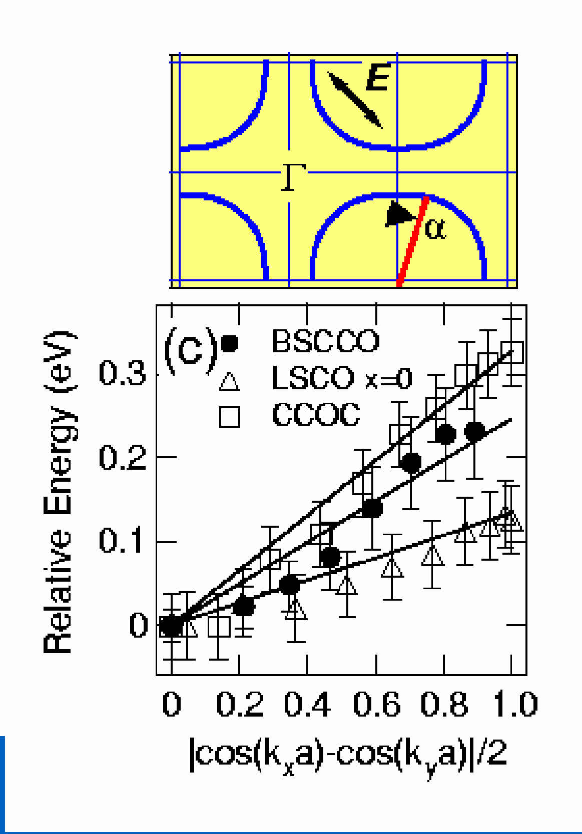



Moraghebi, Moreo, et al., PRL

Mayr et al.

# Dispersion along underlying "Fermi surface" in insulator

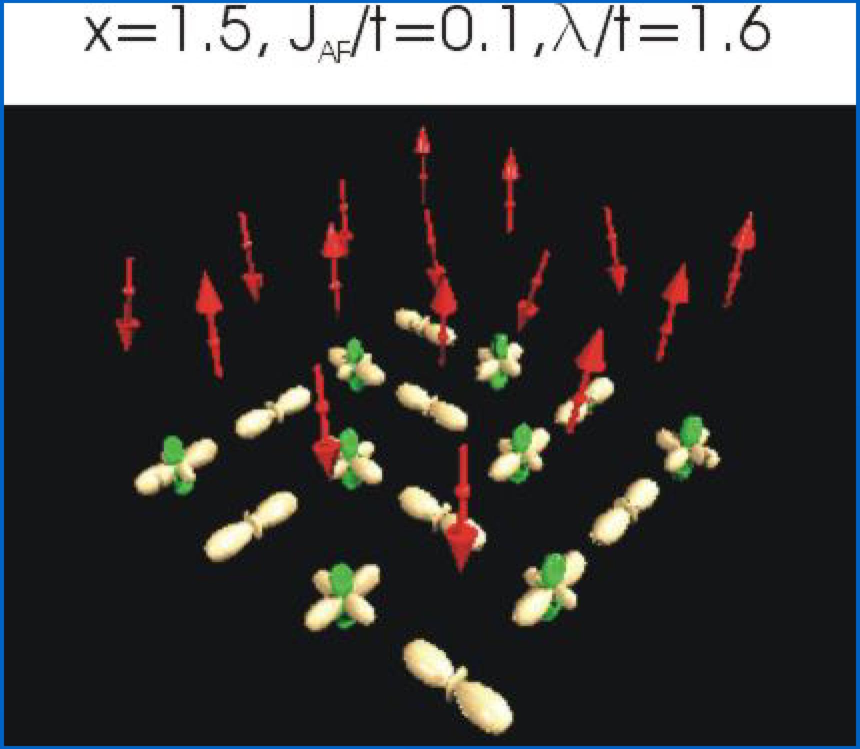



$E(\pi/2,\pi/2) - E(\pi,0) \propto |t'|$

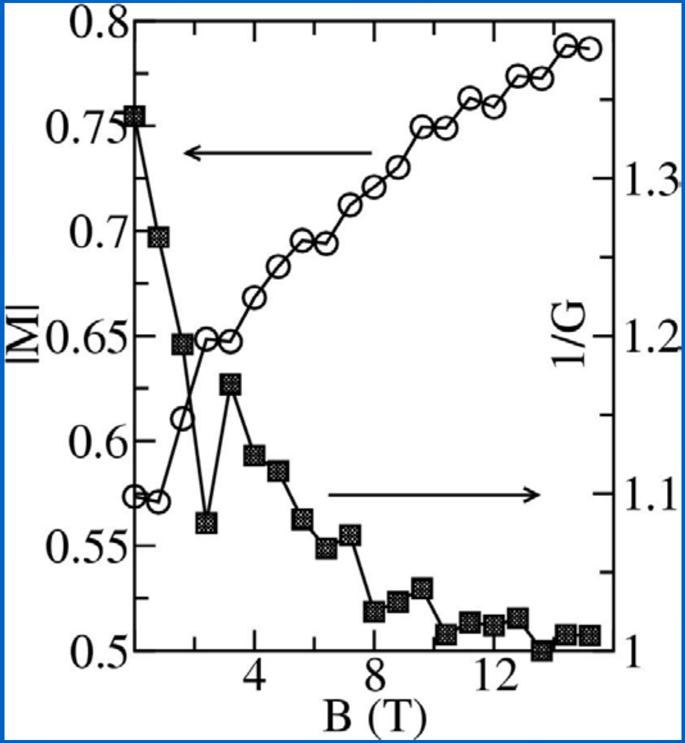
# New: n=1.5 charge-ordered states in electron-doped LaMnO3

Aliaga et al.




Mn(3+)/Mn(2+) CO state

# Large MR in DMS materials?


As in manganites, here the preformed FM regions lead to a robust MR of about 50% at 8T.

t=0.3 eV, J=t

Experiments?